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An Attempt to Estimate Measurement Uncertainty in the Air Force Toxic Chemical Dispersion (AFTOX) Model

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AN ATTEMPT TO ESTIMATE MEASUREMENT UNCERTAINTY IN THE AIR FORCE TOXIC CHEMICAL DISPERSION (AFTOX) MODEL

Abstract

The Air Force Toxic Chemical Dispersion (AFTOX) model is a Gaussian puff dispersion model that predicts plumes, concentrations, and hazard distances of toxic chemical spills. A measurement uncertainty propagation formula derived by Freeman *et al.* (1986) is used within AFTOX to estimate resulting concentration uncertainties due to the effects of data input uncertainties in wind speed, spill height, emission rate, and the horizontal and vertical Gaussian dispersion parameters, and the results are compared to true uncertainties as estimated by standard deviations computed by Monte Carlo simulations.

The measurement uncertainty propagation formula was found to overestimate measurement uncertainty in AFTOX-calculated concentrations by at least 350 percent, with overestimates worsening with increasing stability and/or increasing measurement uncertainty.

Results from the Monte Carlo simulations indicate that during most scenarios, AFTOX is most sensitive to wind speed measurement error, whose contribution to total measurement uncertainty is at least double that of any of the five other

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measurement inputs considered. Spill height is most important close to the source during stable conditions, and during neutral conditions, the contribution by Sigma-X, the horizontal dispersion parameter along the x-axis, is significant. Contributions by remaining parameters are minimal. Concentration measurement uncertainty increases proportionally with increasing data input error.

Monte Carlo simulations are recommended to estimate data input error effects on predicted concentrations in Gaussian puff models simulating continuous releases. Testing of the Freeman *et al.* (1986) formula using an AFTOX-simulated instantaneous release could yield different conclusions.

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THE FLORIDA STATE UNIVERSITY

COLLEGE OF ARTS AND SCIENCES

AN ATTEMPT TO ESTIMATE MEASUREMENT UNCERTAINTY IN THE AIR FORCE TOXIC CHEMICAL DISPERSION (AFTOX) MODEL

By

MARK D. ZETTLEMOYER

A Thesis submitted to the
Department of Meteorology in partial
fulfillment of the requirements for
the degree of Master of Science

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The members of the Committee approve the thesis of Mark D. Zettlemoyer on 10 April 1990.

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AN ATTEMPT TO ESTIMATE MEASUREMENT UNCERTAINTY
IN THE
AIR FORCE TOXIC CHEMICAL DISPERSION (AFTOX) MODEL

Mark D. Zettlemoyer
The Florida State University, 1990

Major Professor: Paul H. Ruscher, Ph.D.

The Air Force Toxic Chemical Dispersion (AFTOX) model is a Gaussian puff dispersion model that predicts plumes, concentrations, and hazard distances of toxic chemical spills. A measurement uncertainty propagation formula derived by Freeman *et al.* (1986) is used within AFTOX to estimate resulting concentration uncertainties due to the effects of data input uncertainties in wind speed, spill height, emission rate, and the horizontal and vertical Gaussian dispersion parameters, and the results are compared to true uncertainties as estimated by standard deviations computed by Monte Carlo simulations.

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overestimates worsening with increasing stability and/or increasing measurement uncertainty.

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Monte Carlo simulations are recommended to estimate data input error effects on predicted concentrations in Gaussian puff models simulating continuous releases. Testing of the Freeman *et al.* (1986) formula using an AFTOX-simulated instantaneous release could yield different conclusions.

DEDICATION

This work is dedicated to the memory of Dr. Thomas A. Carney, who with his passing from this world in October 1989, left behind a legacy of thoughtfulness and caring about others, a zest for learning, and enjoyment of life that touched countless people at Florida State University, in Tallahassee, and beyond. The scientific community lost a dedicated instructor and researcher; his family and friends, a true brother; and the community at large, a man with a big heart who always thought of, and gave freely of himself, to others.

ACKNOWLEDGEMENTS

I am deeply indebted to Catherine Watson, whose work with AFTOX and the measurement error propagation formula laid the groundwork for this research. Her and Dr. Carney's efforts in incorporating the measurement error formula into AFTOX saved me untold hours of computer coding.

Dr. Carney, to whom this work is dedicated, initially stirred my interest in transport and boundary layer processes, and despite failing health, guided me down the initial path of my research.

Many thanks also go to Dr. Paul Ruscher, who was willing to step in after Dr. Carney's passing and provided astute suggestions to organize and plot my data, helped with the manuscript, and lent an ear as we sorted out numbers and what direction to take the research, and to Dr. Steven Hanna, whose insights, from concentration distribution functions to puff behavior, kept my mind on the science involved in my work, rather than on numeric results. I also appreciate Dr. Steven Stage's and Dr. David Stuart's commenting on the thesis.

Lastly, and most lovingly, I want to thank my wife Gloria, for her helpful suggestions, review of the manuscript, and constant interest and encouragement.

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List of Symbols

C.....CONC, an AFTOX model variable representing the predicted chemical concentration for a specified set of inputs

DC.....DCONC, an AFTOX model variable representing the measurement uncertainty calculated by the measurement error propagation formula

G.....chemical concentration at a place and time

h.....effective spill height above ground level

M.....median concentration calculated by 200 runs of AFTOX with six randomized inputs

N_i.....random numbers used in Monte Carlo simulation

SD.....Monte Carlo-generated standard deviation used to estimate true measurement uncertainty

σ_x.....SX or Sigma-X, the standard deviation of G in the x-direction

σ_y.....SY or Sigma-Y, the standard deviation of G in the y-direction

σ_z.....SZ or Sigma-Z, the standard deviation of G in the z-direction

Q.....emission rate (used in AFTOX scenario)

Q(t').....mass of puff at emission

S_G.....standard deviation or measurement uncertainty of a calculated concentration

S_x.....standard deviation or measurement uncertainty of a specified model input

t'.....time of emission (of chemical puff). t-t' is the elapsed time since emission

u.....wind speed at height 10 m

x.....downwind axis, along plume centerline

x_i, x_j...data inputs assumed to have measurement uncertainty associated with them

y.....horizontal axis perpendicular to plume axis, with y=0 at the plume axis

z.....height above the (uniform) ground

I. Introduction

It has long been recognized that dispersion models would be more useful to decision makers if the uncertainty associated with model predictions were quantified. This information could then be used as an additional input into the decision-making process, thus improving confidence in decisions made based on modelling results. But, according to Hanna *et al.* (1988), there are no standard, objective, quantitative means of evaluating currently available microcomputer-based hazard response models. Hanna *et al.* (1988) further point out that a number of such models have recently been proposed and some developed that include up-to-date algorithms on such important scientific phenomena as evaporative emissions, dense gas slumping, and transition from buoyant to non-buoyant dispersion; unfortunately, few data sets exist for testing these models. To date, many models have not been tested or compared against these data using standard statistical significance tests, though concern about quantifying

model uncertainty has led researchers such as Hanna (1989) and Freeman *et al.* (1986) to begin such work.

The uncertainty associated with a particular dispersion model estimate can be divided into three categories (*e.g.*, Gardner and O'Neill, 1983; Freeman *et al.*, 1986):

1) Model formulation uncertainty, resulting from the inadequate description of the modelled event by simplified model parameterizations;

2) Stochastic uncertainty due to the random nature of the atmospheric processes responsible for transport and dispersion; and

3) Measurement uncertainty, resulting from the inherent imprecision or inaccuracy of meteorological instruments, and human interpretation and input error. Hanna (1988) also says that excellent equipment accuracy can be downgraded due to unrepresentative placement of the instrument or inappropriate application of the data.

For the convenience of this research, the first two categories will be grouped together as "model" uncertainty, since both represent possible shortcomings in the model's representation of the actual physics involved in the dispersion process. In general, model uncertainty is believed to be much greater than

measurement uncertainty (Freeman *et al.*, 1986), except perhaps under very stable planetary boundary layer conditions when observations do not neatly "fit" any similarity functions. Some estimates of total uncertainties in model results have been derived, based on the differences between modelled events predicted by simplifying assumptions and observations (*e.g.*, Turner, 1970; Pasquill, 1974). Most researchers have thus attempted to quantify model formulation uncertainty while comparatively few have incorporated measurement uncertainty into model results. However, it may be possible to infer measurement uncertainty in dispersion models from some model sensitivity studies. Freeman *et al.* (1986) reference a number of pertinent model sensitivity analyses and propose an analytical method of incorporating measurement uncertainties into dispersion models.

The United States Air Force (USAF), among others, has placed increased emphasis on calculating accurate toxic corridors due to the potential release of hazardous chemicals. The Ocean Breeze/Dry Gulch (OB/DG) model, originally used for calculating these corridors, does contain an estimate of model uncertainty, but it does not account for important physical phenomena such

as those mentioned previously. Kunkel (1988), under contract work for the USAF, developed an improved model, the Air Force Toxic Chemical Dispersion (AFTOX) model, that includes algorithms for such phenomena as buoyant or non-buoyant dispersion and evaporative emissions. AFTOX, though more advanced scientifically than OB/DG, does not include an estimate of model uncertainty. Kunkel (1988) did include confidence limits on the length of the hazard distance and the concentrations along plume centerline computed by AFTOX, but there are no estimates of what portion of the hazard distance or concentration is uncertain due to model or measurement errors.

The current study examines how measurement uncertainty associated with six input variables propagates through the AFTOX model. The decision to estimate measurement error uncertainty within AFTOX was influenced by research being conducted by Sigma Research Corporation, Westford, Massachusetts, which in July 1987 was awarded a USAF small-business grant to study hazard response modelling uncertainty. The Sigma researchers indicated that studies focusing on measurement rather than modelling uncertainty would be the most complementary, and least redundant, approach. The Air

Force's Air Weather Service distributed Zenith 100 and 200 series microcomputer versions of AFTOX, written in the BASIC language, to its field units in 1989 after its development at the Air Force Geophysics Laboratory (AFGL); consequently, users of the model are far removed from the considerations Kunkel (1988) used in its design, and quantification of the propagation and magnitude of both model and measurement uncertainty in this model should be particularly valuable to decision makers.

II. The Air Force Toxic Chemical Dispersion (AFTOX) Model

Kunkel (1988) based AFTOX on a model called SPILLS, developed by the Shell Oil Company (Fleischer, 1980), but he made several modifications to the code, the more important of which include: the method for computing the atmospheric stability; the use of a continuous stability parameter instead of discrete Pasquill stability categories; the method of summing the concentrations of overlapping puffs; the addition of surface roughness which affects the rate of dispersion; and, the addition of concentration averaging time. Additionally, the program is user-friendly, with only minimal knowledge of the computer and the model required.

AFTOX asks the user to input such environmental parameters as wind speed and direction, temperature, cloud cover and type, ground conditions (wet, dry, snow-covered), and inversion presence, as well as the chemical and type of release involved. Although it

contains a library of 76 chemicals, it may be run for chemicals the user inputs. The program offers a choice of output options, including the concentration at a selected point in space and time, the maximum concentration at a specified elevation and time, or a plot of concentration contours the user selects. The model handles continuous or instantaneous, liquid or gas, releases, and can predict the dispersion of a continuous buoyant plume from a stack as well. Flow charts of processes modelled in AFTOX are in Appendix A.

AFTOX uses a Gaussian puff model that assumes the released mass is conserved during the transport and diffusion process; *i.e.*, there is no deposition or decay. For an instantaneous release, the model follows a single puff as it moves downwind. Though physically unrealistic, puff formulations reasonably predict concentrations when the chemical release time is short relative to the time of travel to points of interest. AFTOX simulates a continuous release by assuming four puffs are released per minute, with the total number of puffs then dependent upon the duration of the chemical release. Continuous releases, particularly from industrial smokestacks, are typically modelled with a Gaussian plume equation (Hanna *et al.*, 1982):

$$G/Q = \{2\pi\sigma_y\sigma_z u\}^{-1}\{\exp(-y^2/2\sigma_y)^2\} \quad (1)$$
$$\times \{\exp(-(z-h)^2/2\sigma_z^2) + \exp(-(z+h)^2/2\sigma_z^2)\}$$

The puff formulation of AFTOX is slightly different from the plume expression:

$$G(x,y,z,t-t') = \{Q(t')/(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z\} \quad (2)$$
$$\times \{\exp(-(x-u(t-t'))^2/2\sigma_x^2)\}$$
$$\times \{\exp(-y^2/2\sigma_y^2)\}$$
$$\times \{\exp(-(z-h)^2/2\sigma_z^2)+\exp(-(z+h)^2/2\sigma_z^2)\}$$

where,

G - chemical concentration at a place and time

t' - time of emission

t-t' - elapsed time since emission

Q(t') - mass of puff at emission

u - wind speed at height of 10 m

σ_x - standard deviation of G in x-direction

σ_y - standard deviation of G in y-direction

σ_z - standard deviation of G in z-direction

x - downwind axis, along plume centerline

y - horizontal axis perpendicular to plume axis, with y=0 at the plume axis

z - height above the (uniform) ground

h - effective height above ground level

The effective height h is found by adding the height of the source above the ground (the release height) to

the distance a buoyant plume rises before it begins to move downwind; for non-buoyant plumes, such as shall be examined here, the effective height is the release height. Sigma-X and Sigma-Y, commonly called the horizontal dispersion or spread parameters, are set equal in AFTOX, thus producing a circular horizontal puff cross-section. All three spread parameters are dependent on atmospheric stability, downwind distance, concentration averaging time, and the roughness length of the site, and were empirically derived from experiments designed for continuous plume considerations (*e.g.*, Barr and Clements, 1984), rather than for puff considerations. Consequently, discrepancies may occur when the standard Pasquill-Gifford disperion parameters are used in puff models such as AFTOX, introducing some bias into the models. This bias might properly be regarded as part of the total uncertainty and outside the focus of this work; however, it will be useful to consider how measurement errors are propagated differently by the respective formulations (*i.e.*, results from the Gaussian plume model examined by Freeman *et al.* (1986) will be contrasted to this study's results).

Rather than use discrete Pasquill stability categories, Kunkel incorporated a continuous stability parameter within AFTOX ranging from 0.5 to 6 to prevent sharp changes in hazard distance when going from one stability category to another, which can happen with slight changes in wind speed, solar angle, or cloud cover. AFTOX uses one of two methods (Mitchell, 1982 or Golder, 1972) to determine these continuous stability parameters, which correspond to Pasquill's categories as follows:

Table 1. Relation between the Pasquill stability categories (SC), AFTOX continuous stability parameters (SP), and the corresponding atmospheric conditions.

SC	A	B	C	D	E	F
SP	0.5-1	1-2	2-3	3-4	4-5	5-6
	extremely unstable			neutral		moderately stable

Stabilities within AFTOX for this research are directly specified, so dispersion and measurement uncertainty for differing atmospheric conditions can be considered.

The last term added together within {brackets} in AFTOX's Gaussian puff formula (2) represents that portion of the plume that is reflected off the ground to rejoin the plume. AFTOX also has an option to calculate dispersion under inversion conditions, but measurement

uncertainty under that meteorological regime is not considered in this study.

In the appropriate module within the program, AFTOX tracks each puff as it joins the mean flow and disperses. Puffs whose centers are four or more standard deviations (sigma parameters) away from the point of interest downwind are assumed to make no contribution to the concentration at that point. The concentration at a given point is then determined by the number of puffs nearby, their sizes at that time, and the amount of material in the puffs, calculated by equation (2).

Much of the previous work concerned with the propagation of errors in dispersion models has focused on Gaussian plume models (*e.g.*, Simpson and Hanna, 1981; Lewellen *et al.*, 1984). These formulations are most appropriate for continuous elevated sources, such as industrial smokestacks, but chemical spills such as could occur on Air Force bases have typically been more successfully modelled with Gaussian puff algorithms. This research seeks to find if an analytical formula used by Freeman *et al.* (1986) accurately estimates the effects of measurement uncertainties propagating through AFTOX, to determine at what point or under which

conditions that formula breaks down within the Gaussian puff formulation of AFTOX, and to quantify measurement uncertainty in the model.

III. Methodology

A. The Measurement Error Propagation Formula

The following equation for the propagation of data input error derived by Freeman *et al.* (1986) is used to examine the uncertainty in computed concentrations from AFTOX associated with specified uncertainties in some input variables:

$$S_G^2 = \sum_{i=1}^{n} (\delta G/\delta x_i)^2 (S_{xi})^2 + \sum_{i=1}^{n} \sum_{j=1}^{n} (\delta^2 G/\delta x_i \delta x_j)^2 (S_{xi})^2 (S_{xj})^2 + 1/2 \sum_{i=1}^{n} (\delta^2 G/\delta x^2{}_i)^2 (S_{xi})^4 \quad (3)$$

where x_i and x_j represent the variables assumed to have known uncertainties upon which the concentration G is dependent (*i.e.*, the first and second order partial and cross-partial terms), the S_x's represent the standard deviation or measurement uncertainty of each variable, and S_G is the uncertainty or standard deviation of the calculated concentration. Equation (3) comes from expanding G in a Taylor series, retaining terms only of second order or less.

The assumptions inherent to the propagation formula (3) are (Freeman *et al.*, 1986):

1) All measurement inputs except the parameters specified for the equation are known exactly;

2) Errors in the specified parameters are random, uncorrelated, and normally distributed with means equal to zero and standard deviations as specified for the propagation equation; and

3) The third and higher terms of the Taylor expansion of G around the true values of the specified parameters are negligible with respect to the first and second order terms, which are assumed to adequately estimate measurement uncertainty for lower (<40%) data input uncertainties. The equation assumes both $(\delta G/\delta x_i)^2(S_{xi})^2$ and $(\delta^2 G/\delta x_i \delta x_j)^2(S_{xi})^2(S_{xj})^2$ are much less than one, an important limitation, since otherwise the sum of the terms calculating the uncertainty will rapidly approach or exceed 100% of the concentration. This assumption does not appear to hold true for the formula's calculations within AFTOX, as will be discussed in Chapter IV. For higher measurement uncertainties S_{xi} (>70%), neglect of higher order terms of the Taylor expansion could cause the formula to underestimate measurement uncertainty error.

The second assumption is also unlikely to be representative for the application of equation (3) to AFTOX. The lower boundary of the input parameters is zero, so a skewed distribution may be more representative than a normal one, especially for stable to very stable conditions. In fact, Irwin *et al.* (1987) suggest that a log-normal distribution is more appropriate. In addition, the uncertainty among some of the specified parameters might be correlated; for example, wind speed helps determine stability, which in turn affects the horizontal and vertical dispersion parameters, so u and each sigma parameter are not uncorrelated. Freeman *et al.* (1986) further discuss specific considerations of parameter uncertainty.

The six AFTOX variables assumed to have known measurement uncertainties are:

1) Source strength Q;

2) Wind speed u;

3) Effective source height h; and

4) Gaussian horizontal and vertical diffusion parameters σ_x, σ_y, and σ_z.

Wind speed is likely to be routinely measured at most USAF sites using AFTOX, and current calibration specifications for USAF weather instrumentation can

provide an estimate of the error associated with such measurements. For example, the current wind measuring equipment used at Air Force bases, a pole-mounted cup anemometer called the AN/GMQ-20, can have measurement errors of 10% to 20% (Fisher *et al.*, 1987). The wind speed, u, of the dispersion equation is, more specifically, the representative transport wind. AFTOX has routines to adjust the input wind speed to be more representative of the transport wind if, for example, the available wind measurement is at an inappropriate height. Such routines introduce additional uncertainty, but the assumption made for the purpose of this study is that the total uncertainty in the input parameters considered, wind speed in this case, is known and thus can be specified *a priori*. Likewise, since not all variables can be directly measured (*i.e.*, the Gaussian spread parameters, although AFTOX does use concentration averaging time and roughness length inputs to adjust these values), it is also presumed that these variables, measured and empirically derived from experimental data, have uncertainties that can be specified *a priori*.

For this work, the uncertainty in each of the variables Q, u, h, and the dispersion parameters has been selected to be 10%, 20%, 30%, and 40% of the input

value. AFTOX prompts the user to input Q, u, and h, and the Gaussian spread parameters are already known from prior AFTOX runs. Downwind distances are assumed to be precisely known, in contrast to the earlier study by Freeman *et al.* (1986), who parameterized relative distance in terms of wind speed and direction, both of which were assigned uncertainties. The uncertainty values chosen are thought to represent reasonable, and perhaps even conservative, measurement errors for these parameters.

B. Use of the Error Propagation Formula and Randomized Inputs in the AFTOX Model

The Freeman *et al.* (1986) error propagation formula, incorporated into AFTOX's Gaussian puff formula algorithm, diagnoses resultant concentration uncertainties under varying stability conditions, which are then compared to concentrations and standard deviations calculated using a Monte Carlo approach to randomize the six aforementioned AFTOX variables. Two separate codings of AFTOX were modified, one to accept measurement uncertainties S_{xi} and use the measurement error propagation formula to determine calculated

concentration uncertainty (the partial derivatives used are listed in Appendix B), and the other to accept randomized deviations to any or all of the parameters Q, u, h, and the Gaussian spread parameters. For both codings, four cases with uncertainties of 10%, 20%, 30%, and 40% were simulated for each combination of AFTOX stability classes 1.5, 2.5, 3.5, and 4.5 and downwind distances of 100, 500, and 1000 meters, with all variables changing uncertainties individually or simultaneously. Environmental conditions and variable uncertainties for the "base case" of 10% are found in Table 2.

For the Monte Carlo simulation, for each combination of stability and distance, normally distributed random numbers N_i with zero mean and a standard deviation of one were used to generate four sets of 1000 input data values for Q_i, u_i, h_i, σ_{xi}, σ_{yi}, and σ_{zi}, where:

Table 2a. Spill corridor parameters.

Latitude/Longitude: 30°N, 80°W
Roughness Length: 10 cm
Height of wind measuring equipment: 12.8 m
Elevation (MSL): 3.05 m

Table 2b. AFTOX input variables that play no significant role in uncertainty calculations due to specified stability classes.

Parameter	Comments
Date of spill: 1 April (90) Time of spill: 1200L	Date and time affect solar elevation angle and heat flux, thus stability
Temperature: 25°C	
Wind direction: 120°	Significantly contributed to measurement error in Freeman *et al.* (1986) study
Cloud cover and type: 3/8, middle (Ac, Sc, Cu)	Cover and type affect heat flux, thus stability
Ground condition: dry	
Inversion: none	

$$Q_i = Q + N_{iQ}S_Q \qquad u_i = u + N_{iu}S_u$$

$$h_i = h + N_{ih}S_h \qquad \sigma_{xi} = \sigma_x + N_i\sigma_x S\sigma_x \qquad (4)$$

$$\sigma_{yi} = \sigma_y + N_i\sigma_y S\sigma_y \qquad \sigma_{zi} = \sigma_z + N_i\sigma_z S\sigma_z$$

and S_a represents the uncertainty or standard deviation of the subscripted variables above, set to 10%, 20%, 30%, or 40%.

All data sets with randomly-deviated AFTOX inputs were screened to eliminate non-positive values (physically unrealistic) and variable values more than four standard deviations from the mean value. All deviations generated by the Box-Muller method (Press *et*

Table 2c. Environmental variables and uncertainties used in AFTOX "base case" runs.

Parameter	Uncertainty	Comments
Stabilities: 1.5, 2.5, 3.5, 4.5		Input directly. Affects sigma values.
Downwind distances: 100m, 500m, 1000m		Affects sigma values. Crosswind distance = 0
Area of spill: 0 sq m		Gas release (NO_3) is a point source.
Spill site roughness length: 3 cm		AFTOX adjusts sigma values.
Amount emitted: 10 kg/min	1 kg/min, 10%	Continuous release.
Spill height: 5 meters	.5 m, 10%	
Elapsed time since spill: 10 minutes		AFTOX determines number of puffs.
Concentration averaging time: 10 minutes		AFTOX adjusts sigma values.
Wind speed: 5 meters/sec	.5 m/s, 10%	Important AFTOX input; affects stability, sigma values, etc.
Sigma parameters	10% for each	Inputs controlled to yield same values for each run.

al., 1986) applied to BASIC's random number generator, and subsequently added to the AFTOX inputs above, were used. Two hundred of these random deviations were then

bootstrapped (sampling with replacement; see Hanna, 1989) from each file, unique for its particular combination of uncertainty, stability, and downwind distance, and added to the base value of each variable, thus computing 200 concentrations and a variance for each combination of these three parameters. Although Freeman *et al.* (1986) used 2500 input data values for each combination of parameters, Fischer *et al.* (1988) justified the use of sample sizes of 100 and 200 for Monte Carlo simulations. Statistical t-tests done on runs of 10, 20, 50, 100, 200, 500, and 1000 calculated concentrations indicated that as low as 50 AFTOX runs would have yielded acceptable (95% confidence level) mean, median, and standard deviation values.

This randomized-input version of AFTOX was run under the conditions shown in Table 2 to generate 200 predicted concentrations for every possible combination of measurement uncertainty, distance, and stability. The median concentrations and standard deviations of these Monte Carlo sets are compared with the corresponding concentrations and measurement error formula-calculated uncertainties found by running the other modified AFTOX program, to determine at what level(s) of measurement uncertainty the Freeman *et al.*

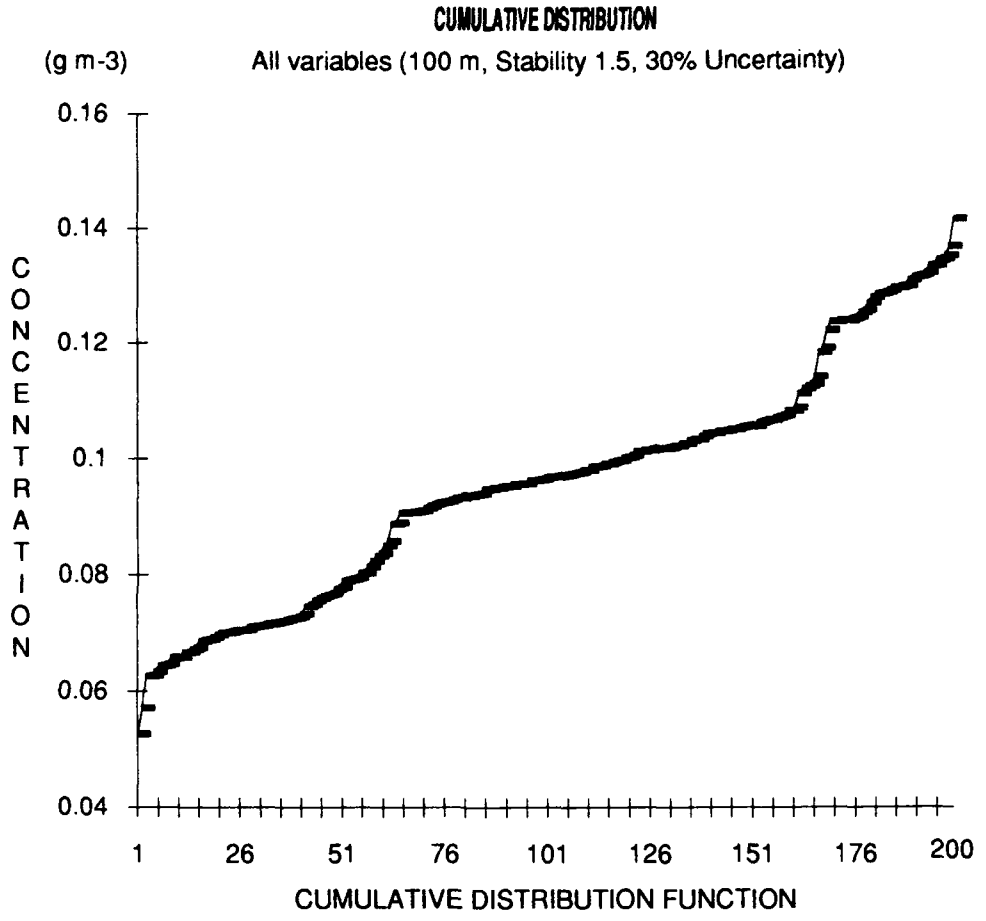
(1986) error formulation reasonably predicts measurement error propagating through this Gaussian puff model. Formula-calculated uncertainties are examined relative to the corresponding model-derived concentrations as appropriate, to estimate how measurement error affects chemical concentrations computed by AFTOX, and the results are contrasted with those of Freeman *et al.* (1986).

IV. Results and Discussion

A. Comparison of Error Formula and Monte Carlo Uncertainties

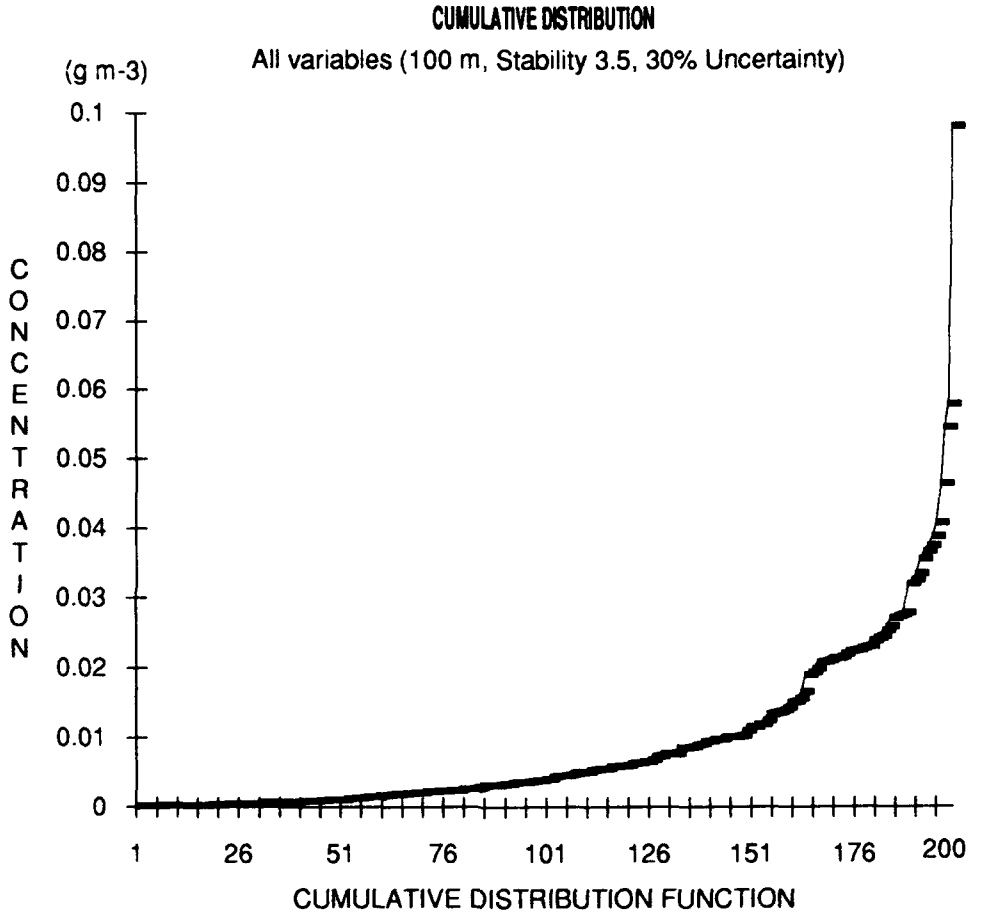
Model predicted concentrations (C) and their associated uncertainties calculated by the measurement error propagation formula (DC) when using the "base case" inputs (Table 2) are compared with the median concentrations (M) and standard deviations (SD) of model predictions calculated from the Monte Carlo simulations for AFTOX stabilities 1.5, 2.5, 3.5, and 4.5. This analysis differs from that of Freeman *et al.* (1986), since median rather than mean concentrations from the Monte Carlo runs are used, and the compared downwind distances are different. Additionally, some stabilities specified in AFTOX are physically unattainable in the model for the input conditions prescribed.

The cumulative distribution functions (cdf's, Figures 1 and 2) depict the range of concentrations calculated with all inputs varying at once, for 100 m downwind, 30% measurement uncertainty, and stabilities of 1.5 (moderately unstable) and 3.5 (neutral). Most



Mean concentration = 0.0960 g/m^3
Median concentration = 0.0968 g/m^3
AFTOX-calculated concentration = 0.1006 g/m^3

Figure 1. Cumulative Distribution Function of Monte Carlo-generated concentration values with six AFTOX inputs changing simultaneously, for 100 m downwind, moderately unstable conditions, and 30% measurement uncertainty.



Mean concentration = 0.0091 g/m^3
Median concentration = 0.0041 g/m^3
AFTOX-calculated concentration = 0.0028 g/m^3

Figure 2. Cumulative Distribution Function of Monte Carlo-generated concentration values with six AFTOX inputs changing simultaneously, for 100 m downwind, neutral conditions, and 30% measurement uncertainty.

cdf's of the Monte Carlo files looked like that of Figure 1, with concentrations distributed approximately normally, and with the mean, median, and actual AFTOX-generated concentration values within 5% of each other. However, a few of the distributions looked like that of Figure 2. Concentrations for this scenario were generally less than 0.01 g/m^3, but with a few outlying values that raised the mean of the distribution and resulted in the median concentration more closely approximating the "base case" concentration. Therefore, median concentrations were used for all ensuing analyses.

The second disparity between this research and that of Freeman *et al.* (1986) is that they reported results for downwind distances of 3, 7, and 15 km, while this research uses distances of 100, 500, and 1000 m. Since Kunkel (1988) coded AFTOX to report only three significant digits for predicted concentrations with units of parts per million or mg/m^3, concentrations far beyond one kilometer are forecast to be 0 mg/m^3. AFTOX was not altered to forecast the smaller concentrations far downwind. Freeman *et al.* (1986) did report contributions to total variance by each varied input parameter at the distances used here for AFTOX, but no

other data was immediately available for 100, 500, and 1000 m downwind.

Another important point to consider is the stabilities used for this research. Freeman *et al.* (1986) used stabilities A, B, C, and D in the Environmental Protection Agency's Industrial Source Complex Short Term (ISCST) Gaussian plume model (see Table 1), but they did not discuss how ISCST computes atmospheric stability, nor if all the stabilities they used are physically attainable by the model for the given inputs. For the current set of AFTOX inputs, the model computes an atmospheric stability of 2.5 using Golder's (1972) method. Randomized deviations to the wind speed could result in stabilities of 2.14 to 2.68, if the base wind speed is deviated to 4 or 6 m/sec; otherwise, additional inputs into AFTOX must be changed to expand the range of potential possible stabilities (Table 3). Specifying stabilities thus avoided the need to change other inputs to get the desired stabilities within AFTOX. This is important, because for a noontime spill under partly cloudy skies with a wind speed of 5 m/sec, the atmosphere is likely to be slightly unstable. In the AFTOX runs done here, it is desired to do the calculations for the same input conditions. In order to

observe in the atmosphere, or for AFTOX to simulate, slightly stable (AFTOX stability 4.5) conditions, the initial input variables would have to have been substantially altered (refer to Table 3, 0000L and clear

Table 3. Varying AFTOX inputs[1] and resultant stabilities.

Time of Spill (local time)	U (m/sec)	Cloud Cover	Cloud Type	Resulting Stability
0800L	5	0/8	---	3.08
		3/8	mid	3.04
		8/8	low	3.50
1200L	4	0/8	---	2.14
		3/8	mid	2.14
		8/8	low	3.23
1200L	5	0/8	---	2.50
		3/8	*mid*	*2.50*[2]
		8/8	low	3.36
1200L	6	0/8	---	2.69
		3/8	mid	2.68
		8/8	low	3.41
0000L	4	0/8	---	4.45
		3/8	N/A[3]	4.06
		8/8	N/A	3.50
0000L	5	0/8	---	3.98
		3/8	N/A	3.75
		8/8	N/A	3.50

Notes:
1. All other inputs as listed in Table 2.
2. Stability resulting from current set of AFTOX inputs.
3. Not applicable since cloud cover is not an AFTOX input during nighttime.

skies.

Freeman *et al.* (1986) reported that the error propagation formula they used in the ISCST model estimated the "true" measurement uncertainty, as approximated by the standard deviations computed by the Monte Carlo simulations, to within 25% for most stabilities, downwind distances, and measurement uncertainties. The notable exception occurred during neutral conditions, when the error formula overestimated measurement uncertainty by as much as 216% (15 km downwind, neutral stability, 40% measurement uncertainty). The error formula (3), when applied to AFTOX's puff formulation, consistently overestimated the true measurement uncertainty propagating through the model (Table 4). Possible reasons for this will be discussed later. At best, the error formula overestimated the true uncertainty by 350%. Despite the significant overestimation, the error formula illustrates that measurement uncertainties propagating through AFTOX increase significantly with increasing data input uncertainty. Not unsurprisingly, measurement uncertainties were highest for stability 4.5, slightly stable conditions, an atmospheric regime which is currently difficult to describe in dispersion model

Table 4. Ratio of calculated to true uncertainty (DC/SD) as a function of stability, downwind distance, and magnitude of input data uncertainty. Six variables uncertain simultaneously.

Downwind Distance	Stability Class	Measurement Uncertainty 10%	20%	30%	40%
100 m	1.5 (B)	14.3	9.0	13.6	21.0
	2.5 (C)	7.5	7.9	11.7	18.8
	3.5 (D)	3.5	5.9	10.1	15.0
	4.5 (E)	703.3	1377.6	1805.9	2391.6
500 m	1.5 (B)	6.2	10.0	11.8	16.9
	2.5 (C)	13.6	22.1	26.9	43.3
	3.5 (D)	30.2	44.5	63.8	87.2
	4.5 (E)	39.9	82.5	141.5	170.7
1000 m	1.5 (B)	4.1	6.8	9.4	10.9
	2.5 (C)	7.2	11.9	18.2	25.1
	3.5 (D)	19.9	36.3	49.6	71.2
	4.5 (E)	69.1	124.4	170.6	240.9

algorithms.

Analysis of the ratios of calculated concentrations to the Monte Carlo method's median concentrations provides a means to determine if data input uncertainty is likely to cause a model to underestimate or overestimate the resulting concentration for a particular stability. In the Freeman *et al.* (1986) study, the ratios of model-calculated concentrations to Monte Carlo mean concentrations were close to unity for 10% data input uncertainty, with a systematic divergence as uncertainties increased. Again, a notable

overestimate occurred during neutral conditions, when measurement uncertainties caused the ISCST model to overpredict the resulting concentration by as much as 158% (15 km downwind, 40% data input uncertainty).

The effects of different stabilities on dispersion are evident in Table 5. During unstable conditions, with vigorous vertical motions occurring in the atmosphere, concentrations should be higher close to the elevated source than further downwind, as particles are rapidly mixed to the surface. On the other hand, during neutral and stable conditions, pollutants remain suspended in the atmosphere for a longer time before settling to the ground, and dispersion and deposition should result in higher concentrations farther downwind than close to the source. AFTOX-calculated concentrations agree with this general, physical interpretation of dispersion.

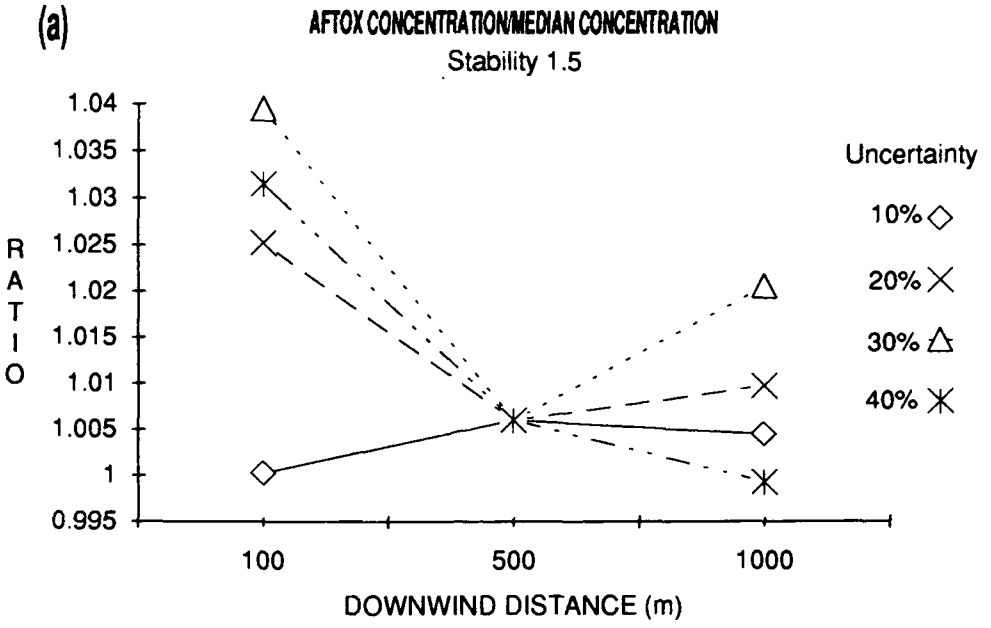
Table 5. AFTOX-calculated concentrations (g/m^3) as a function of stability and downwind distance.

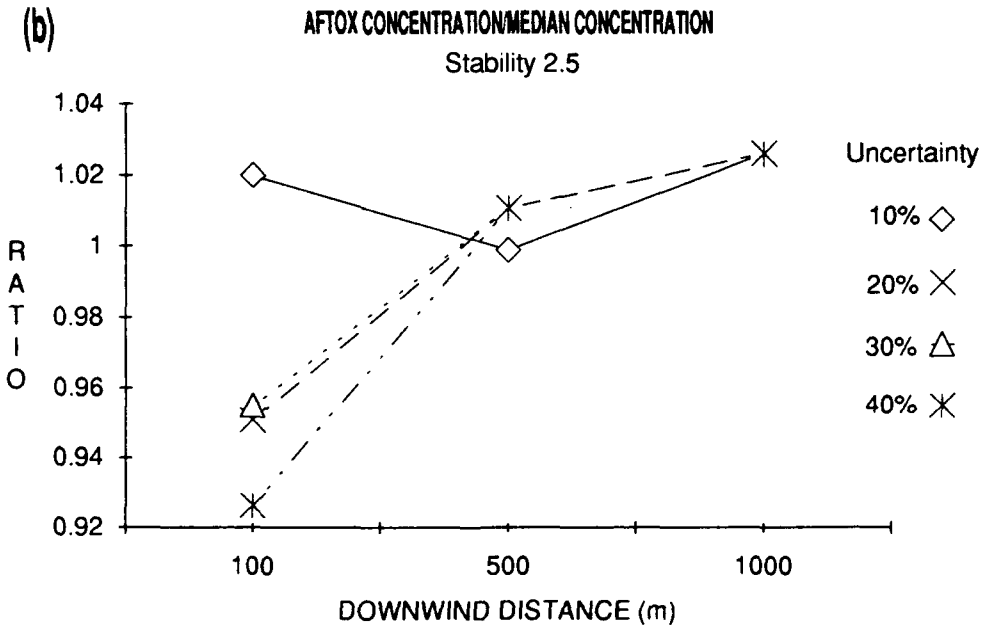
Downwind Distance	Stability 1.5	2.5	3.5	4.5
100 m	0.1006	0.1332	0.0028	0.0003
500 m	0.0037	0.0084	0.0218	0.0392
1000 m	0.0010	0.0024	0.0072	0.0152

Unlike the Freeman *et al.* (1986) results, data input errors do not cause AFTOX to significantly overpredict or underpredict concentrations (Table 6 and Figures 3), though close to the source the AFTOX-calculated concentrations are underestimated by up to 30% during neutral conditions (Figure 3c, 100 m), when compared to the Monte Carlo-generated median concentrations. Data input errors also cause AFTOX to overestimate concentrations by 15% for measurement uncertainty of 40% during a slightly stable regime. This is attributable to the fact that 100 m is the limit of AFTOX's accuracy-

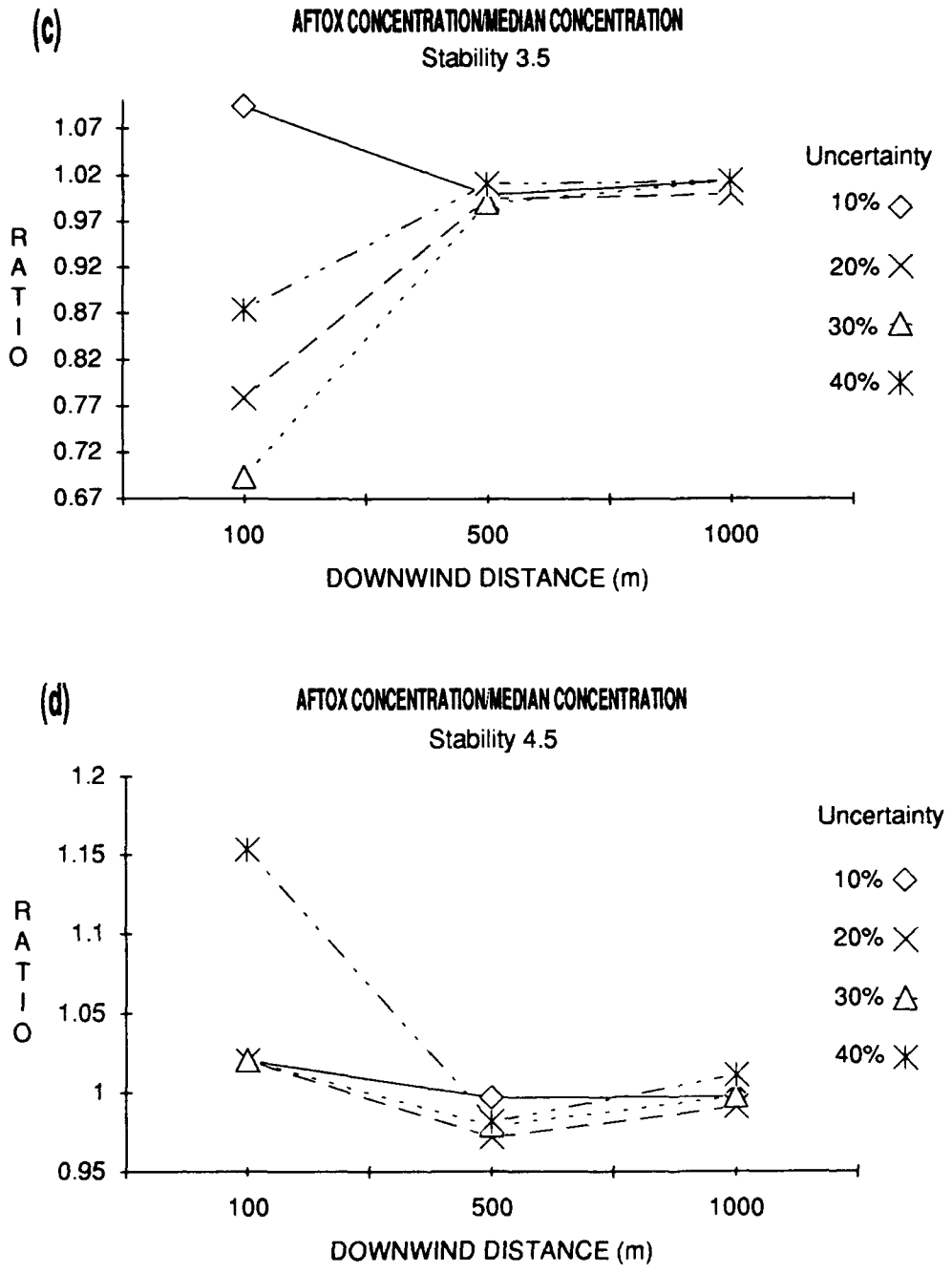
Table 6. Ratio of concentration to median (C/M) as a function of stability, downwind distance, and magnitude of data input uncertainty. Six variables uncertain simultaneously.

Downwind Distance	Stability Class	Measurement Uncertainty 10%	20%	30%	40%
100 m	1.5 (B)	1.000	1.025	1.040	1.032
	2.5 (C)	1.020	0.951	0.955	0.926
	3.5 (D)	1.094	0.779	0.694	0.875
	4.5 (E)	1.020	1.020	1.020	1.153
500 m	1.5 (B)	1.006	1.006	1.006	1.006
	2.5 (C)	0.999	1.011	1.011	1.011
	3.5 (D)	1.000	0.995	0.991	1.012
	4.5 (E)	0.997	0.972	0.980	0.982
1000 m	1.5 (B)	1.005	1.010	1.021	0.999
	2.5 (C)	1.026	1.026	1.026	1.026
	3.5 (D)	1.013	0.999	1.013	1.013
	4.5 (E)	0.998	0.991	0.998	1.011





Figures 3a, 3b. The ratios of Concentration/Median plotted for each downwind distance and measurement uncertainty within the specified stability regime.



Figures 3c, 3d. The ratios of Concentration/Median plotted for each downwind distance and measurement uncertainty within the specified stability regime.

it will not allow the user to compute a concentration closer than 100 m to the source. As subsequent analysis will show, the ratio of the part of the concentration that is uncertain due to measurement uncertainties to the calculated concentration is highest at 100 m during neutral and slightly stable conditions. Measurement uncertainties affect the calculated concentrations 500 m and 1000 m downwind by 3% or less, a result likely to be true for AFTOX predictions beyond one kilometer, since the results for 500 m and 1000 m are similar.

Tables 7 and 8 depict the relative magnitudes of uncertainties calculated by the error formula (3) and the Monte Carlo-generated standard deviations by giving the ratios of the calculated uncertainty or true uncertainty to the calculated concentration. Freeman *et al.* (1986) reported that for 30% data input uncertainty, the error formula (3) estimated uncertainty of the calculated concentration to be at least 50% of the calculated concentration, and at 40% uncertainty, the calculated uncertainty exceeded the concentration. Results from the error propagation formula in AFTOX estimate that the uncertain portion of the concentration ranges from 9% to 84,207%, an expected result, since the error formula significantly overestimates measurement

Table 7. Ratio of calculated uncertainty to concentration (DC/C) as a function of stability, downwind distance, and magnitude of data input uncertainty. Six variables uncertain simultaneously.

Downwind Distance	Stability Class	Measurement Uncertainty 10%	20%	30%	40%
100 m	1.5 (B)	0.41	1.29	2.74	4.77
	2.5 (C)	0.87	1.96	3.43	5.35
	3.5 (D)	5.95	21.69	47.88	84.54
	4.5 (E)	53.35	211.10	474.00	842.07
500 m	1.5 (B)	0.15	0.45	0.91	1.55
	2.5 (C)	0.33	1.00	2.10	3.62
	3.5 (D)	0.75	2.35	4.94	8.55
	4.5 (E)	1.71	4.82	9.65	16.29
1000 m	1.5 (B)	0.09	0.26	0.54	0.92
	2.5 (C)	0.19	0.61	1.29	2.23
	3.5 (D)	0.48	1.67	3.63	6.36
	4.5 (E)	1.57	5.94	13.20	23.35

uncertainty within AFTOX. Increasing portions of the concentrations are uncertain with increasing stability and data input uncertainty.

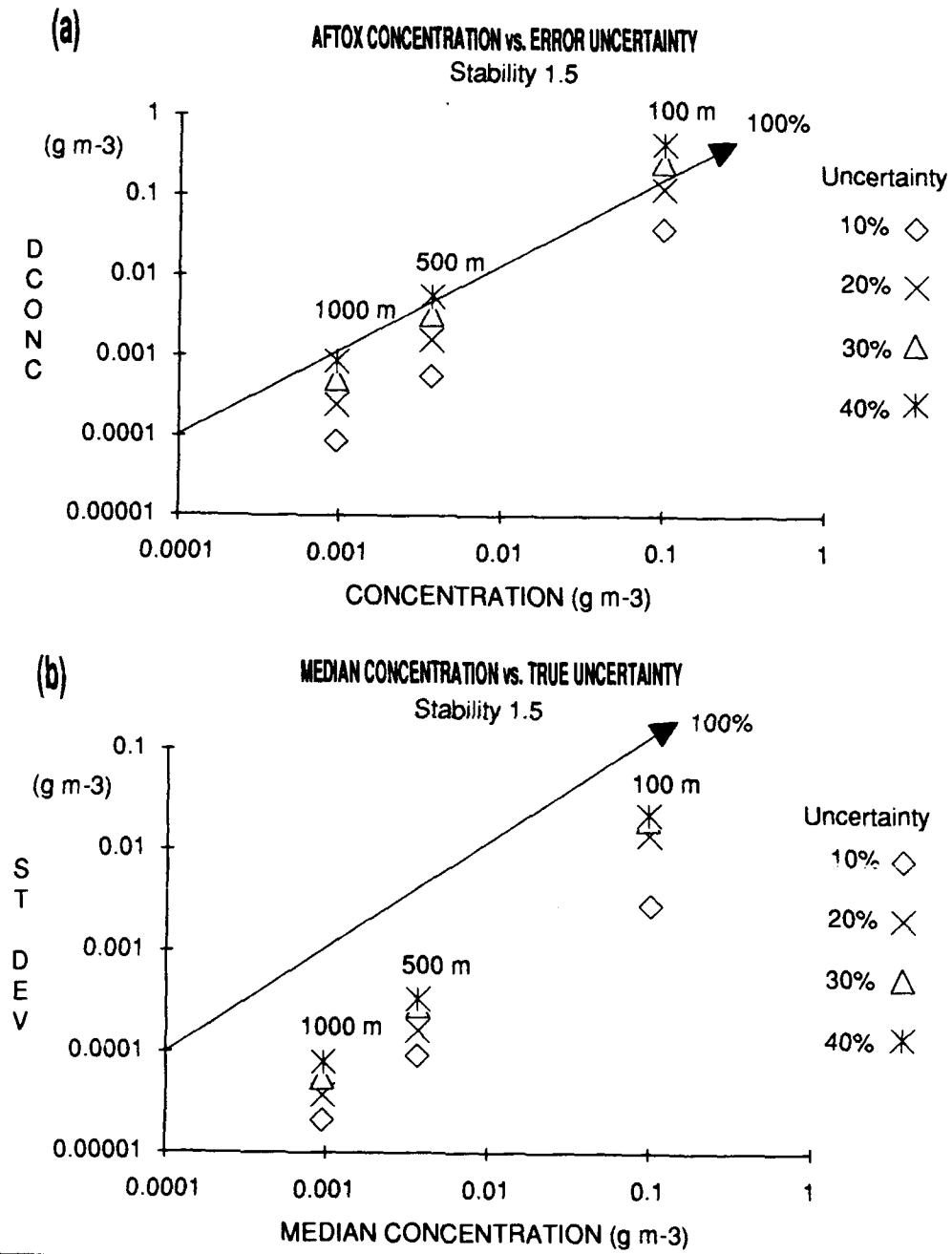
AFTOX appears highly sensitive to data input error close to the source during neutral conditions (Table 8). At 100 m the uncertain portion of the concentration exceeds the calculated concentration, while farther downwind, data input uncertainties of 40% cause less than 10% of each resulting concentration to be uncertain. For stabilities other than 3.5, 30% and higher data input uncertainties cause the resulting

Table 8. Ratio of true uncertainty to concentration (SD/C) as a function of stability, downwind distance, and magnitude of data input uncertainty. Six variables uncertain simultaneously.

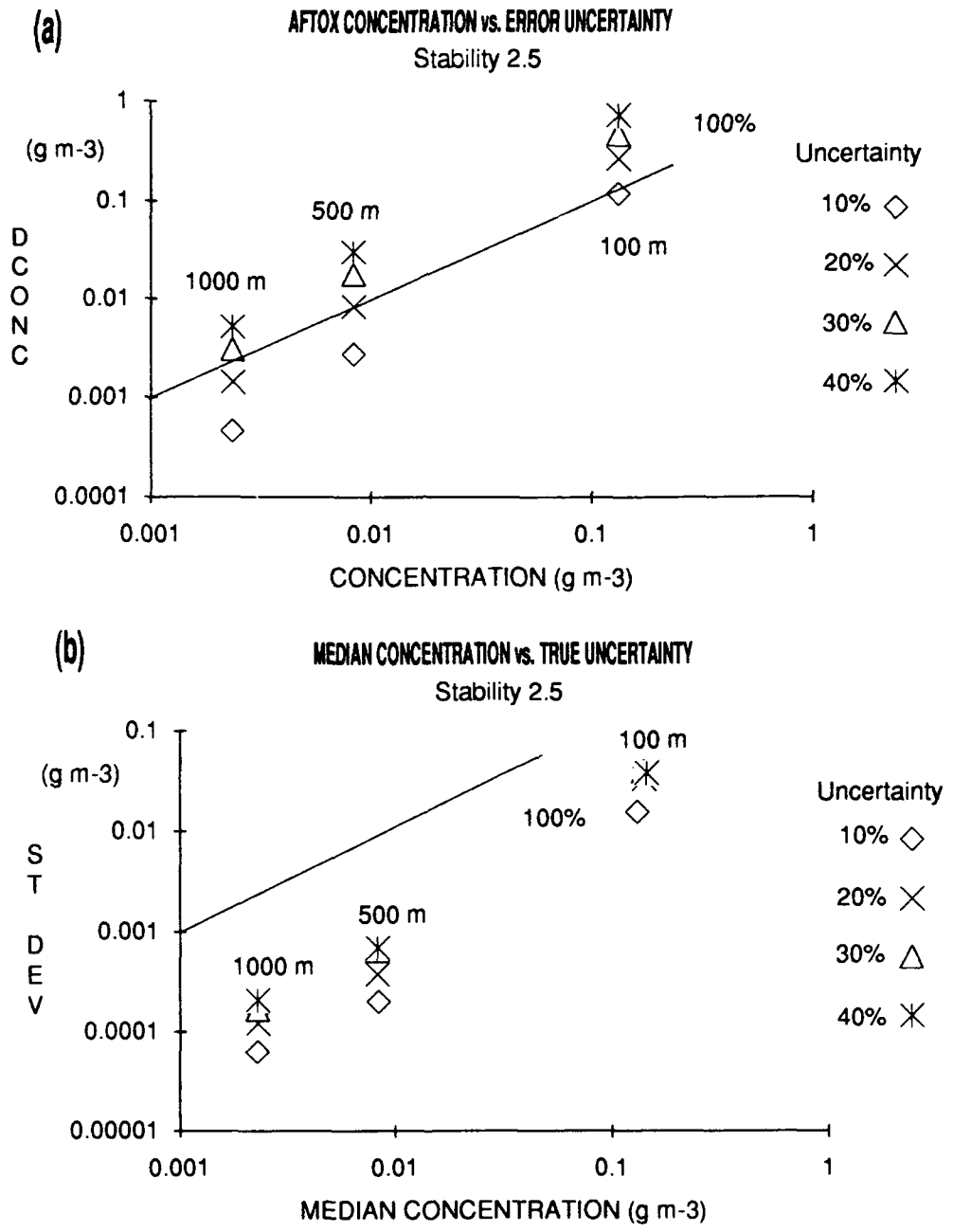
Downwind Distance	Stability Class	Measurement Uncertainty 10%	20%	30%	40%
100 m	1.5 (B)	0.028	0.143	0.201	0.228
	2.5 (C)	0.116	0.248	0.292	0.284
	3.5 (D)	1.688	3.667	4.741	5.632
	4.5 (E)	0.076	0.153	0.262	0.352
500 m	1.5 (B)	0.025	0.044	0.077	0.091
	2.5 (C)	0.024	0.046	0.078	0.084
	3.5 (D)	0.025	0.053	0.077	0.098
	4.5 (E)	0.043	0.058	0.068	0.095
1000 m	1.5 (B)	0.022	0.039	0.057	0.085
	2.5 (C)	0.027	0.052	0.071	0.089
	3.5 (D)	0.024	0.046	0.073	0.089
	4.5 (E)	0.023	0.048	0.077	0.097

concentrations to be 20% to 35% uncertain, which still is a significant portion of the concentration.

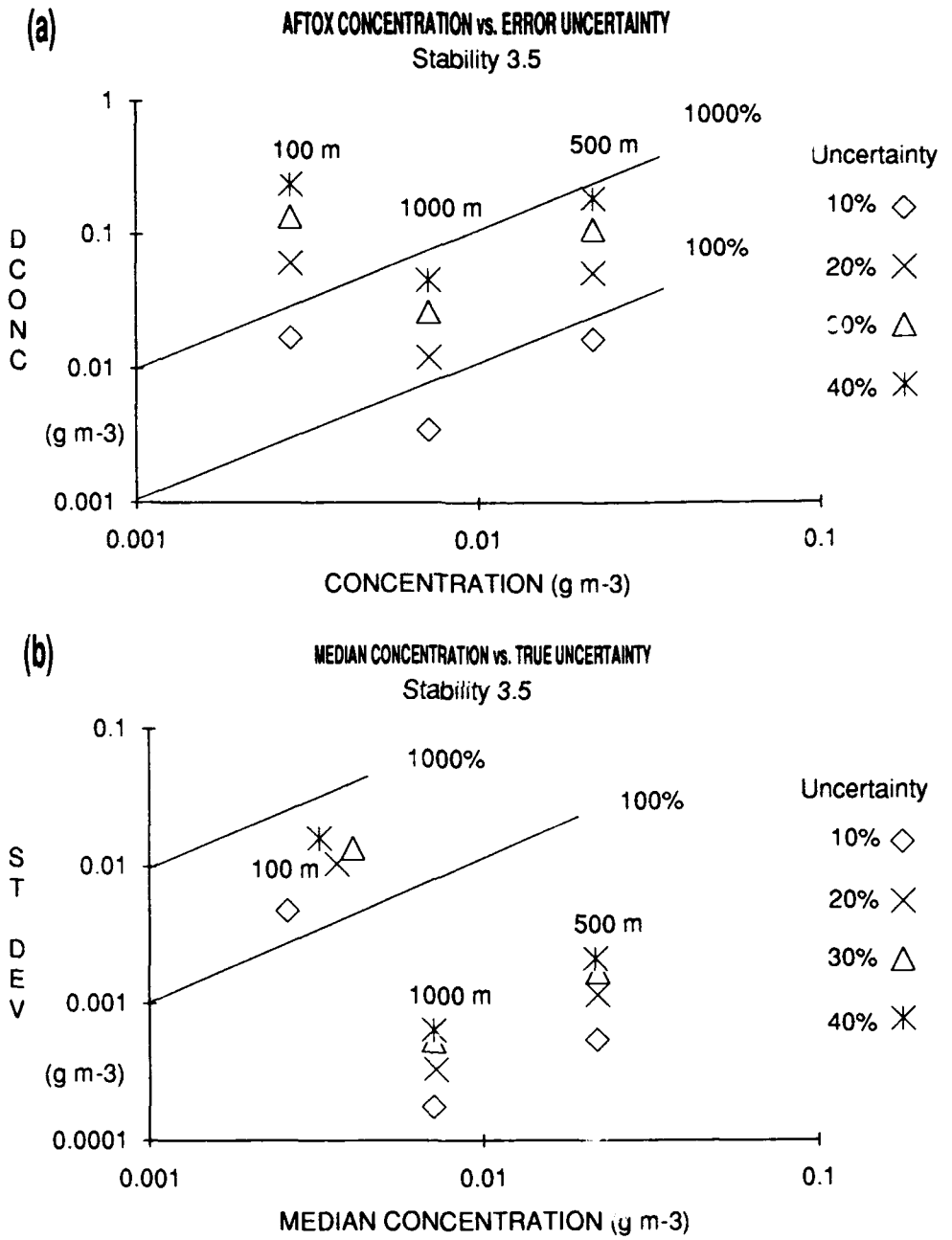
The data used to generate the ratios in Tables 4, 6, 7, and 8 are plotted on logarithmic scales in Figures 4 through 7. The plots illustrate the effects of differing stabilities on dispersion of the chemical, and by using the scales along the axes, it is possible to compare the relative magnitudes of the error formula-calculated uncertainties to AFTOX concentrations and the Monte Carlo-generated standard deviations to the median concentrations. Likewise, the magnitudes of DC values



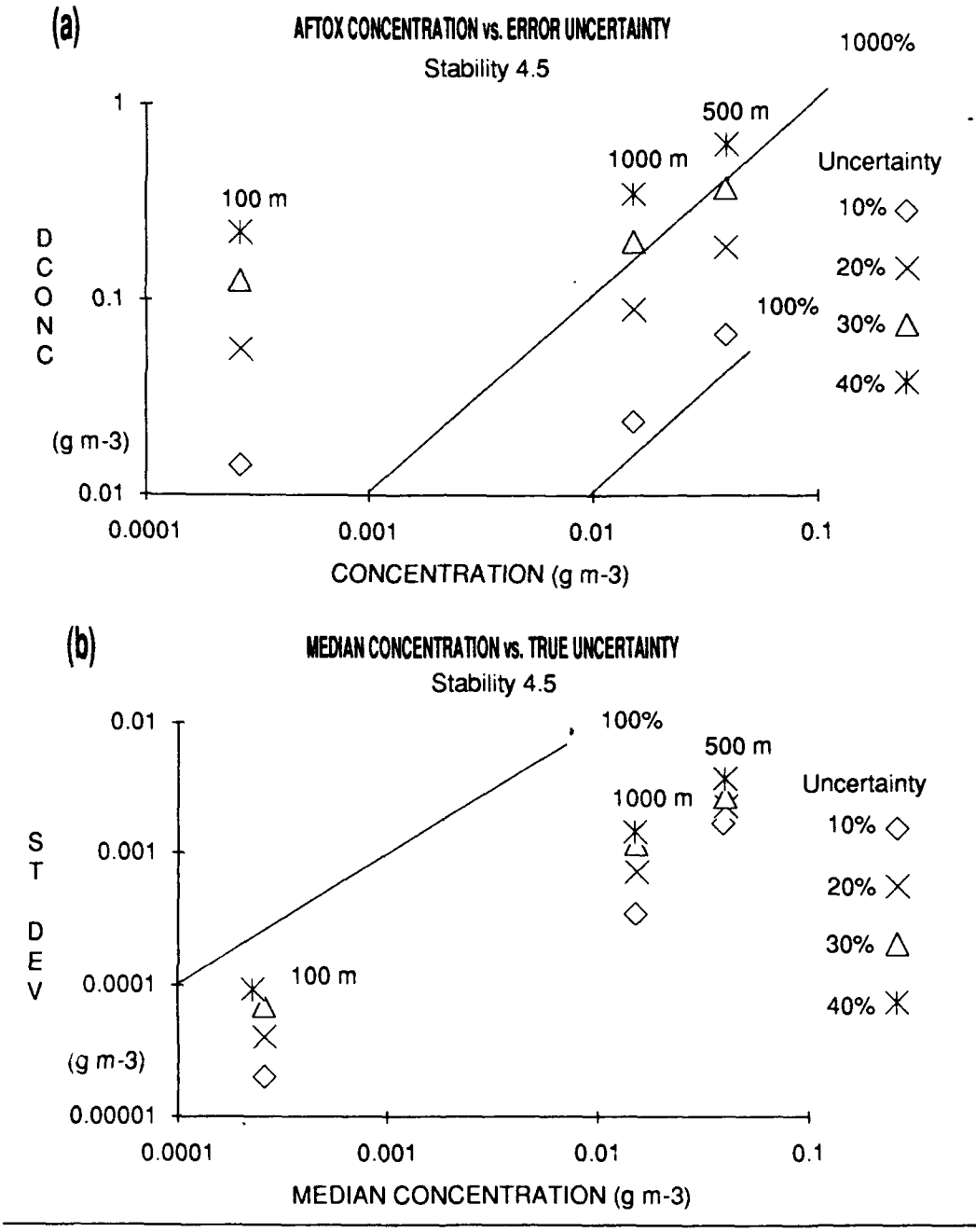
Figures 4a, 4b. Plots of each concentration (4a) or median concentration (4b) versus its corresponding calculated uncertainty (4a) or true uncertainty (4b) for each downwind distance and data input uncertainty within the specified stability regime.



Figures 5a, 5b. Plots of each concentration (5a) or median concentration (5b) versus its corresponding calculated uncertainty (5a) or true uncertainty (5b) for each downwind distance and data input uncertainty within the specified stability regime.



Figures 6a, 6b. Plots of each concentration (6a) or median concentration (6b) versus its corresponding calculated uncertainty (6a) or true uncertainty (6b) for each downwind distance and data input uncertainty within the specified stability regime.



Figures 7a, 7b. Plots of each concentration (7a) or median concentration (7b) versus its corresponding calculated uncertainty (7a) or true uncertainty (7b) for each downwind distance and data input uncertainty within the specified stability regime.

and the corresponding true uncertainties SD can be roughly compared.

The Line of 100% (Figures 4 to 7) is the line along which the calculated uncertain portion of the concentration due to data input uncertainty is equal to the calculated concentration. Similarly, the Line of 1000% shows where the uncertain portion of the concentration is ten times the concentration. These lines can provide a basis for reference when comparing charts.

During unstable conditions (stabilities 1.5 and 2.5), Figures 4 and 5 depict the largest concentrations close to the source and DC approaching and exceeding 100% of the calculated concentration (Figures 4a and 5a), while the true uncertainties SD are about 10% of the Monte Carlo-derived median concentrations (Figures 4b and 5b). The vertical alignment of measurement uncertainties 10% through 40% indicates that increasing data input uncertainty amplifies resulting uncertainty in the predicted concentrations.

During neutral conditions, the high uncertainty of the calculated concentrations at 100 m is immediately evident (Figure 6). The error formula estimates the uncertain portion of the concentration (DC) to be over

1000% of the concentration, and even the Monte Carlo runs suggest that AFTOX results under these conditions are over 100% uncertain due only to data input uncertainties. Downwind, however, the standard deviations indicate that the uncertain portions of the concentrations are still of order 10%. The overestimation of true measurement uncertainty by the error formula is evident by comparing Figures 6a and 6b.

Figure 7 shows the error formula dramatically overestimating concentration uncertainties, as calculated uncertainties DC are approximately 1000% of the concentrations, while the true uncertainties SD continue to be about 10% of each median concentration at any downwind distance.

The data reported and plotted thus far reflect AFTOX runs when wind, spill height, emission rate, and the dispersion parameters simultaneously contained measurement input uncertainties of the same value; *e.g.*, 10%, 20%, 30%, or 40%. Additional error formula and Monte Carlo runs varied just one measurement input at a time, in order to examine the relative contributions of each parameter to the final measurement uncertainty.

B. Relative Contributions of Each Measurement Input to Measurement Uncertainty

Freeman *et al.* (1986) found measurement uncertainties in the measured wind direction to be the largest contributor to the total measurement uncertainty of calculated concentrations for their Gaussian plume simulations. Wind direction, though, is not an explicit parameter in the Gaussian plume equation (1), as written. The downwind and crosswind distances, x and y, are expressed as functions of the wind direction vector in the Freeman *et al.* (1986) study, with downwind locations specified such that they are aligned along the mean wind direction. The inputted deviations from this mean wind direction, representing measurement uncertainty, would then cause the plume centerline to be off the x-axis some distance, y', related to the angle of deviation. Thus the relationship of each downwind distance reported by Freeman *et al.* (1986) to the mean transport wind should also be affected by the specified deviations in the wind direction. Freeman *et al.* (1986) did not report how they parameterized these effects, so

that the partial derivatives in the error propagation equation (3) could be taken. For this reason, concentration uncertainty due to measurement uncertainty of the wind direction was not evaluated for the AFTOX model.

Freeman *et al.* (1986) concluded that uncertainty in the measured wind direction of 3^{o} contributes over 40% of the total measurement uncertainty for distances beyond two kilometers. The Gaussian spread parameters are the next largest contributors, with emission height important only close to the source and wind speed (1% to 3%) and source strength (2 to 6%) contributing little to the total variance.

In the Gaussian puff formulation of AFTOX, however, wind speed appears in the exponential term that represents the spread and transport of a puff along the x-axis. When the partial derivative of the concentration G is taken with respect to u (see Appendix B), it becomes an important source of uncertainty in the measurement error propagation equation (3) and an important contributing factor to the overestimation of measurement uncertainty by equation (3). Likewise, nonlinearities due to exponential terms involving the sigma terms and height of the spill caused some

calculated concentration distributions to be other than normally distributed (Figure 2), although the randomized inputs were normally distributed. The puff algorithm of AFTOX also causes equation (3) to overestimate measurement uncertainty by adding the uncertainty of puffs close to the point of interest.

AFTOX uses its puff formula, equation (2), to compute the concentration of each puff whose center is within four horizontal and vertical dispersion parameters of the puff concentrations upwind and downwind of the point of interest, then sums all contributing concentrations to predict the concentration at a point in space and time (Kunkel, 1988). Within AFTOX, the error formula (3) computes each puff's standard deviation or measurement uncertainty, then multiplies this value by the puff concentration, producing a weighted average representative of that puff's relative contribution to the total measurement uncertainty. Contributions by all puffs are summed to find DCONC (DC), the portion of the concentration that is uncertain due to measurement uncertainty. Although puffs are physically unrealistic, the sum of the concentrations of overlapping puffs yields a reasonable predicted concentration, but the summing of DCONC values

could compound overlapping but correlated uncertainties, resulting in the error formula (3) overestimating the effects of measurement uncertainty within AFTOX.

This discussion will emphasize relative contributions by wind speed (u), spill height (h), emission rate (Q), and the Gaussian spread parameters (SX, SY, and SZ) to measurement uncertainties calculated by the Monte Carlo method, since error formula (3) estimates of DC are high, though DC figures are provided for reference and comparison. Relative contributions to measurement uncertainty by each input were evaluated by running AFTOX with just that parameter having data input uncertainty. A classic analysis of variance to compute each variable's contributions to uncertainty while all variables are changing at once and cross-correlations are accounted for was not done, again due to AFTOX's complexity and research time constraints.

Each AFTOX input contributes to concentration measurement uncertainty with varying degrees of importance, based on downwind distance, stability, and data input uncertainty (Tables 9 and 10). The ratios of each parameter's estimated and true measurement uncertainty values to the calculated concentrations reflect the percentage of the concentration that is

uncertain due to data input uncertainties in only that specific parameter.

Of the six data inputs considered, wind speed is in most circumstances the most important parameter contributing to measurement uncertainty (Tables 10a, 10b, and 10c). Its contribution to total measurement uncertainty due to its input errors is at least double any other parameter, with the lone exception being close to the source (100 m) during slightly stable conditions,

Table 9a. Ratio of calculated uncertainty to concentration (DC/C) for each AFTOX input as a function of stability and magnitude of data input uncertainty for 100 m downwind, when only the specified input varies.

Stability	Data Error	AFTOX Measurement Input u	h	Q	SX	SY	SZ
1.5 (B)	10%	0.36	0.04	0.10	0.09	0.10	0.06
	20%	1.20	0.08	0.20	0.18	0.21	0.12
	30%	2.60	0.12	0.30	0.28	0.32	0.18
	40%	4.55	0.16	0.40	0.39	0.46	0.24
2.5 (C)	10%	0.81	0.07	0.10	0.02	0.10	0.03
	20%	1.63	0.15	0.20	0.07	0.21	0.06
	30%	2.46	0.22	0.30	0.15	0.33	0.11
	40%	3.32	0.30	0.40	0.26	0.46	0.17
3.5 (D)	10%	5.81	0.13	0.09	0.91	0.09	0.05
	20%	21.29	0.26	0.18	2.21	0.19	0.12
	30%	47.05	0.40	0.27	4.10	0.29	0.22
	40%	83.11	0.53	0.36	6.67	0.41	0.36
4.5 (E)	10%	53.14	0.24	0.10	1.96	0.10	0.14
	20%	210.33	0.49	0.20	5.86	0.21	0.30
	30%	472.30	0.75	0.30	12.19	0.33	0.50
	40%	839.07	1.02	0.40	21.01	0.46	0.73

when spill height is most important (Table 10a, stability 4.5). Generally, as wind speed uncertainty improves from 40% to 10%, there is a similar, proportional decrease in that parameter's contribution to measurement uncertainty.

Sigma-X is the second-most important contributor to measurement uncertainty close to the source, particularly during unstable and neutral conditions

Table 9b. Ratio of calculated uncertainty to concentration (DC/C) for each AFTOX input as a function of stability and magnitude of data input uncertainty for 500 m downwind, when only the specified input varies.

Stability	Data Error	u	AFTOX Measurement Input h	Q	SX	SY	SZ
1.5 (B)	10%	0.14	*	0.02	0.02	0.02	0.02
	20%	0.40	*	0.05	0.04	0.05	0.05
	30%	0.82	*	0.07	0.07	0.08	0.08
	40%	1.39	*	0.10	0.09	0.11	0.11
2.5 (C)	10%	0.31	*	0.03	0.03	0.03	0.03
	20%	0.94	*	0.07	0.05	0.07	0.07
	30%	1.95	*	0.10	0.08	0.11	0.11
	40%	3.35	*	0.14	0.11	0.16	0.15
3.5 (D)	10%	0.72	0.01	0.05	0.03	0.05	0.04
	20%	2.23	0.01	0.09	0.06	0.10	0.08
	30%	4.63	0.02	0.14	0.10	0.15	0.13
	40%	7.96	0.02	0.19	0.14	0.22	0.18
4.5 (E)	10%	1.65	0.01	0.05	0.02	0.05	0.04
	20%	4.43	0.03	0.11	0.06	0.11	0.08
	30%	8.52	0.04	0.16	0.12	0.17	0.12
	40%	13.98	0.05	0.21	0.19	0.24	0.17

* Relative contribution < 0.5%.

(Table 10a). At only 100 m downwind, most puffs are still located along plume centerline and contribute more to the calculated concentration than do the fewer laterally and vertically moving puffs. Farther from the spill, puffs are moving away from the plume axis, thus increasing the contributions of laterally and vertically-positioned puffs. Sigma-Z appears to be more important than Sigma-X at 100 m during stable

Table 9c. Ratio of calculated uncertainty to concentration (DC/C) for each AFTOX input as a function of stability and magnitude of data input uncertainty for 1000 m downwind, when only the specified input varies.

Stability	Data Error	AFTOX Measurement Input u	h	Q	SX	SY	SZ
1.5 (B)	10%	0.08	*	0.01	0.01	0.01	0.01
	20%	0.24	*	0.03	0.02	0.03	0.03
	30%	0.49	*	0.04	0.03	0.04	0.04
	40%	0.82	*	0.05	0.05	0.06	0.06
2.5 (C)	10%	0.19	*	0.02	0.01	0.02	0.02
	20%	0.58	*	0.04	0.03	0.04	0.04
	30%	1.21	*	0.05	0.05	0.06	0.06
	40%	2.08	*	0.07	0.07	0.08	0.08
3.5 (D)	10%	0.47	*	0.03	0.02	0.03	0.03
	20%	1.62	*	0.05	0.04	0.05	0.05
	30%	3.52	*	0.08	0.07	0.08	0.08
	40%	6.16	*	0.10	0.10	0.12	0.11
4.5 (E)	10%	1.56	*	0.04	0.04	0.04	0.04
	20%	5.88	0.01	0.08	0.08	0.08	0.07
	30%	13.06	0.01	0.12	0.13	0.13	0.11
	40%	23.10	0.01	0.15	0.18	0.18	0.16

* Relative contribution < 0.5%.

conditions, but this result is questionable since a stability of 4.5 was specified with the wind speed approximately 5 m/sec, an impossible combination in AFTOX. (The wind speed is approximately 5 m/sec since this input was randomly varied during the Monte Carlo simulation.)

Sigma-Z, with the possible exception noted above, and the other inputs contribute relatively little to

Table 10a. Ratio of true uncertainty to concentration (SD/C) for each AFTOX input as a function of stability and magnitude of data input uncertainty for 100 m downwind, when only the specified input varies.

Stability	Data Error	AFTOX Measurement Input u	h	Q	SX	SY	SZ
1.5 (B)	10%	0.05	0.01	0.01	0.01	0.01	0.01
	20%	0.14	0.02	0.02	0.03	0.01	0.01
	30%	0.19	0.02	0.03	0.04	0.02	0.02
	40%	0.22	0.04	0.04	0.06	0.03	0.03
2.5 (C)	10%	0.10	0.01	0.01	0.04	0.01	*
	20%	0.23	0.03	0.02	0.07	0.02	0.01
	30%	0.28	0.04	0.03	0.12	0.02	0.01
	40%	0.30	0.06	0.05	0.16	0.03	0.02
3.5 (D)	10%	1.35	0.03	0.01	0.25	0.01	0.01
	20%	3.33	0.06	0.02	0.58	0.02	0.03
	30%	3.92	0.09	0.03	0.97	0.04	0.04
	40%	4.16	0.12	0.04	1.82	0.05	0.06
4.5 (E)	10%	0.03	0.05	0.01	0.02	0.02	0.04
	20%	0.08	0.10	0.02	0.04	0.04	0.08
	30%	0.14	0.13	0.03	0.06	0.06	0.13
	40%	0.15	0.21	0.04	0.07	0.07	0.17

* Relative contribution < 0.5%.

the measurement uncertainty. The importance of Sigma-Z slowly increases with increasing stability and measurement uncertainty but in general could be expected to add less than 3% to concentration measurement uncertainty. Similarly, the emission rate Q should constitute less than 5% of the concentration uncertainty, as should Sigma-Y, and the source height's contribution is only important when calculating

Table 10b. Ratio of true uncertainty to concentration (SD/C) for each AFTOX input as a function of stability and magnitude of data input uncertainty for 500 m downwind, when only the specified input varies.

Stability	Data Error	AFTOX Measurement Input u	h	Q	SX	SY	SZ
1.5 (B)	10%	0.02	*	0.02	*	*	*
	20%	0.05	*	0.02	*	0.01	0.01
	30%	0.07	*	0.03	*	0.01	0.01
	40%	0.08	*	0.04	*	0.01	0.01
2.5 (C)	10%	0.02	*	0.01	*	0.01	0.01
	20%	0.04	0.01	0.02	*	0.01	0.01
	30%	0.06	0.01	0.03	*	0.01	0.01
	40%	0.08	0.01	0.04	*	0.01	0.02
3.5 (D)	10%	0.02	*	0.01	*	*	0.01
	20%	0.04	0.01	0.02	*	0.01	0.01
	30%	0.06	0.01	0.03	*	0.01	0.02
	40%	0.09	0.01	0.04	*	0.01	0.03
4.5 (E)	10%	0.04	0.01	0.01	*	*	0.01
	20%	0.05	0.01	0.02	0.01	0.01	0.01
	30%	0.05	0.02	0.03	0.01	0.01	0.02
	40%	0.07	0.02	0.04	0.02	0.02	0.03

* Relative contribution < 0.5%.

concentrations close to the source.

The present results suggest that puff models such as AFTOX will be most sensitive to data input uncertainties in wind speed and relatively insensitive to uncertainties in the other parameters specified in this study. This is fortunate for several reasons: wind speed measurement is the easiest of the variable measurements to improve; an accurate estimate of the

Table 10c. Ratio of true uncertainty to concentration (SD/C) for each AFTOX input as a function of stability and magnitude of data input uncertainty for 1000 m downwind, when only the specified input varies.

Stability	Data Error	AFTOX Measurement Input u	h	Q	SX	SY	SZ
1.5 (B)	10%	0.02	*	0.01	*	*	0.01
	20%	0.04	*	0.02	*	0.01	0.01
	30%	0.05	*	0.03	*	0.01	0.01
	40%	0.08	*	0.04	*	0.01	0.01
2.5 (C)	10%	0.02	*	0.01	*	*	*
	20%	0.05	*	0.02	*	*	*
	30%	0.07	*	0.03	*	*	*
	40%	0.08	*	0.04	*	*	0.01
3.5 (D)	10%	0.02	0.01	0.01	*	0.01	0.01
	20%	0.04	0.01	0.02	*	0.01	0.01
	30%	0.06	0.01	0.03	*	0.01	0.02
	40%	0.08	0.01	0.04	*	0.01	0.02
4.5 (E)	10%	0.02	*	0.01	*	*	0.01
	20%	0.04	*	0.02	*	*	0.01
	30%	0.07	0.01	0.03	*	0.01	0.02
	40%	0.09	0.01	0.04	*	0.01	0.02

* Relative contribution < 0.5%.

amount of chemical spilled or its emission rate is unlikely, at least initially; the height of a spill, if at other than ground level, is probably going to be inaccurately estimated; and, since the dispersion parameters are usually not directly measurable, the indication that these three parameters are less important suggests that differences in model routines for determining their values should not greatly influence the uncertainty of AFTOX's results. Also, since the ratios reported in Tables 10b and 10c are similar, the results suggest that AFTOX and similar puff models should not be overly sensitive to data input errors beyond 500 m.

As pointed out previously, AFTOX was run with specified stabilities, some of which are not possible unless other model inputs are changed. Additionally, AFTOX computed concentrations of NO_3 ten minutes after the start of a *continuous* release. Results might be different if an instantaneous release were considered. Prior work with the error formula and AFTOX continuous releases by Watson and Carney (1987, unpublished manuscript) yielded results similar to those presented here, but their simulations of *instantaneous* releases showed that farther downwind (2500 m), Sigma-Z supplants

wind speed as the most important contributor to measurement uncertainty during the stability regimes studied (1.5, 3.5, and 4.5). They did not verify their results against a Monte Carlo simulation. The measurement error formula (3) could not compound the uncertainty of a series of puffs, as possibly happens for a continuous release, if a one puff, instantaneous release were modelled. Although this study demonstrates the Freeman *et al.* (1986) error formula inadequately estimates measurement uncertainty in a puff-modelled continuous release, a test of error formula results versus a Monte Carlo simulation using an instantaneous release might yield slightly different conclusions.

V. Summary and Recommendations

Kunkel (1988) pointed out in the AFTOX User's Manual that the model's predicted hazard distances and concentrations are mean values, so that half the time AFTOX will overpredict and half the time AFTOX will underpredict the hazard distance or concentration. Using data from the Prairie Grass, Green Glow, Ocean Breeze, and Dry Gulch dispersion experiments, he established correction factors for other than the 50% confidence level. For example, the user must multiply the calculated mean concentration by a factor of seven when AFTOX uses Golder's (1972) method to find stability to be 95% certain the calculated concentration won't be exceeded in reality. Data input uncertainties during certain atmospheric conditions can skew this mean concentration (Figures 1 and 2), so this overall correction factor may or not be correct. Freeman *et al.* (1986) point out that measurement uncertainty is much less than the model concentration uncertainty Kunkel (1988) computed correction factors for; however, they write that it is still worthwhile to estimate how data

input errors affect model output:

> "Regulatory issues associated with air quality model predictions may be discussed more intelligently if models include, along with estimated pollutant concentrations, an estimate of at least the minimum (measurement) uncertainty of those predictions. It is recognized that in most practical applications, the model uncertainty is probably on the order of a factor of 2, at best. One might argue that the measurement uncertainty is negligible compared to model uncertainty and need not be considered. This argument implies, however, that the models probably shouldn't be used at all. In the words of Sklarew[1], 'It is anticipated that the error bounds will be so large for most real-world applications of Gaussian models that the models will be shown to be totally useless!' The fact is that these models *are* used, and they often return results with seven significant digits. The calculation of a measurement uncertainty associated with a model prediction, based on reasonable and widely accepted input data uncertainties, supplies only the *minimum* uncertainty. This is still more realistic than no uncertainty at all."

This inquiry initially sought to use a measurement error propagation formula derived by Freeman *et al.* (1986) within the Air Force Toxic Chemical Dispersion (AFTOX) model to estimate how uncertain calculated concentrations became due to data input errors of six parameters. After comparing the error formula's results to those of a Monte Carlo simulation, in which similar

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[1] Sklarew, R.C., 1979: Atmospheric dispersion modeling, a critical review: discussion papers. J. Air Pollut. Control Assoc., **29**, 935.

AFTOX variables were randomly deviated, it was determined that the analytical approach drastically overestimated measurement uncertainty propagating through the AFTOX model.

The failure by the error formula to calculate reasonable measurement uncertainties, which were estimated by Monte Carlo-derived concentration standard deviations, is probably due to a number of factors. Some stabilities used in this study are physically unrealistic within AFTOX, and not all measurements used in the error propagation formula (3) are uncorrelated. The puff formula of AFTOX contains exponential terms, whose non-linear effects both within the model and in the error formula-required derivatives cause resulting concentration distributions to be non-normally distributed, although the inputted deviations are normally distributed. (The Monte Carlo simulations indicated data input errors will cause AFTOX to underestimate forecast concentrations.) Lastly, for the physically realistic, continuous release simulated here, the error formula's compounding effect of adding uncertainties of overlapping puffs could overwhelm the model-calculated concentrations.

It appears the Freeman *et al.* (1986) error formula is best applied to simpler models than AFTOX, although further study should verify if the formula better estimates measurement uncertainty effects on calculated concentrations in a puff-simulated instantaneous chemical release. Although Monte Carlo simulations such as done in this study or by any of a number of other researchers (*e.g.*, Tiwari and Hobbie, 1976) are computationally intensive, this process better approximates measurement uncertainty in AFTOX than the analytical method introduced by Freeman *et al.* (1986).

The Monte Carlo simulations revealed AFTOX is generally most sensitive to wind speed uncertainty, rather than emission rate, spill height, or dispersion parameter input uncertainties, within one kilometer of the spill site. Measurements of the latter five variables are much more difficult to improve than that of wind speed. AFTOX is also particularly sensitive to measurement uncertainties 100 m downwind of the spill, where the model first allows the user to compute concentrations. Users should be especially aware of wind speed inputs and high concentration measurement uncertainties this close to the source, especially during neutral conditions. Test runs, not reported

here, suggest that during AFTOX stabilities 3-4, calculated concentrations could be overwhelmed by wind speed measurement uncertainty out to 200 m from the source.

AFTOX and the error formula need to be the subject of further study to answer some questions not addressed here. Unanswered questions include:

1) Were results impacted because stabilities were directly specified?

2) Why is AFTOX so sensitive to wind speed close to the source, particularly when the atmosphere is well-mixed (neutral), but not so much so during stable conditions?

3) Is AFTOX sensitive to wind direction, and if so, how much?

4) Could the error formula (3) adequately describe measurement uncertainty during an instantaneous release?

Additionally, a classic analysis of variance could give an indication of how much measured inputs interact with one another, and would yield more accurate information on individual parameter contributions to measurement uncertainty.

As of early 1990, an Air Force weather forecaster, responding to a chemical spill on the base, takes a wind

speed measurement that could be highly inaccurate, especially if winds are light, inputs it and other inexact measurements into a model that is most sensitive to wind speed measurement uncertainty, and gets a calculated concentration that is only 50% certain. That calculated concentration, possibly off by more than a factor of seven, is already partially or completely uncertain, depending on atmospheric conditions. This research has hopefully taken a step towards quantifying that portion of the total uncertainty known as measurement uncertainty contained in that predicted AFTOX concentration.

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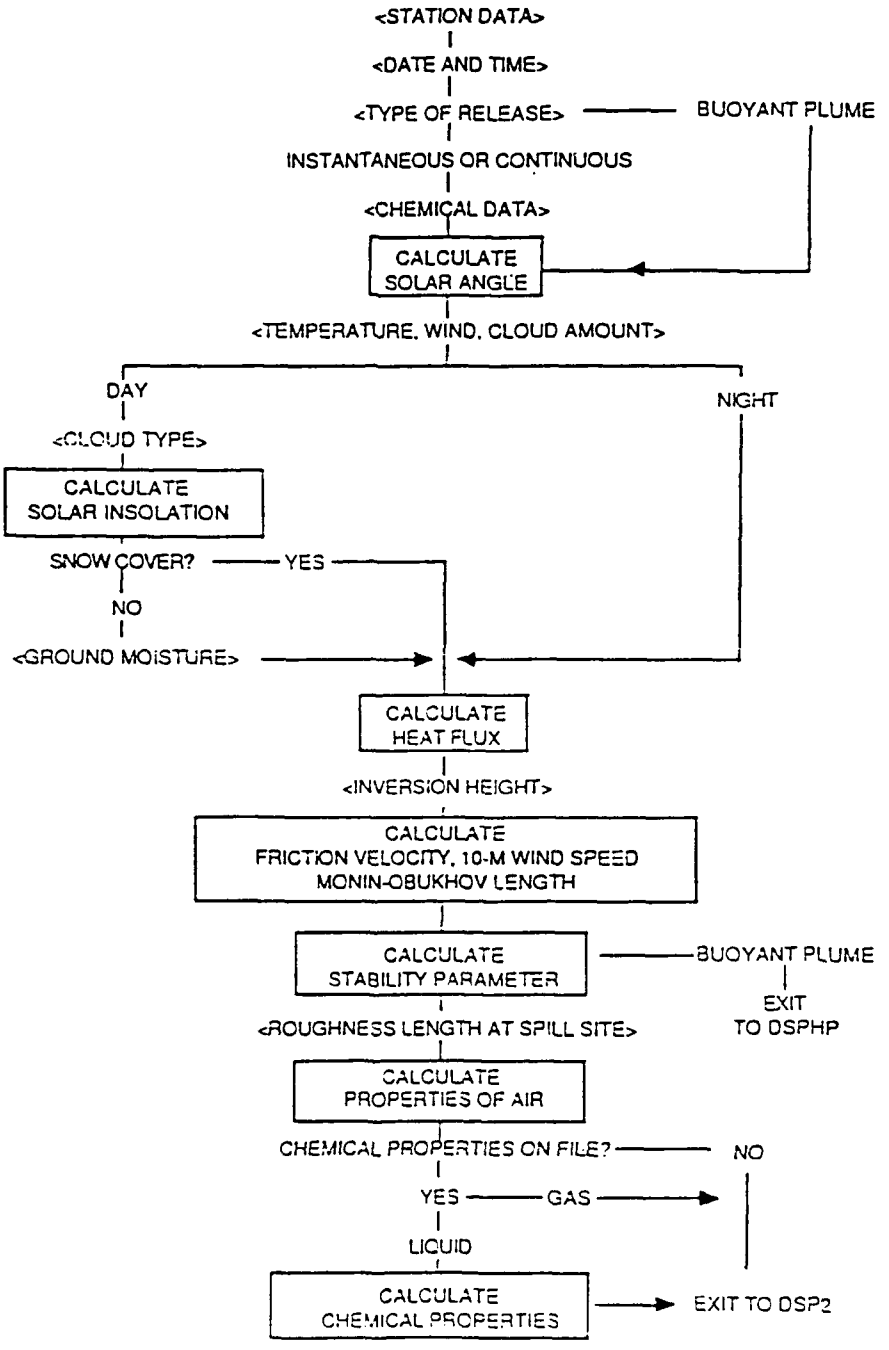
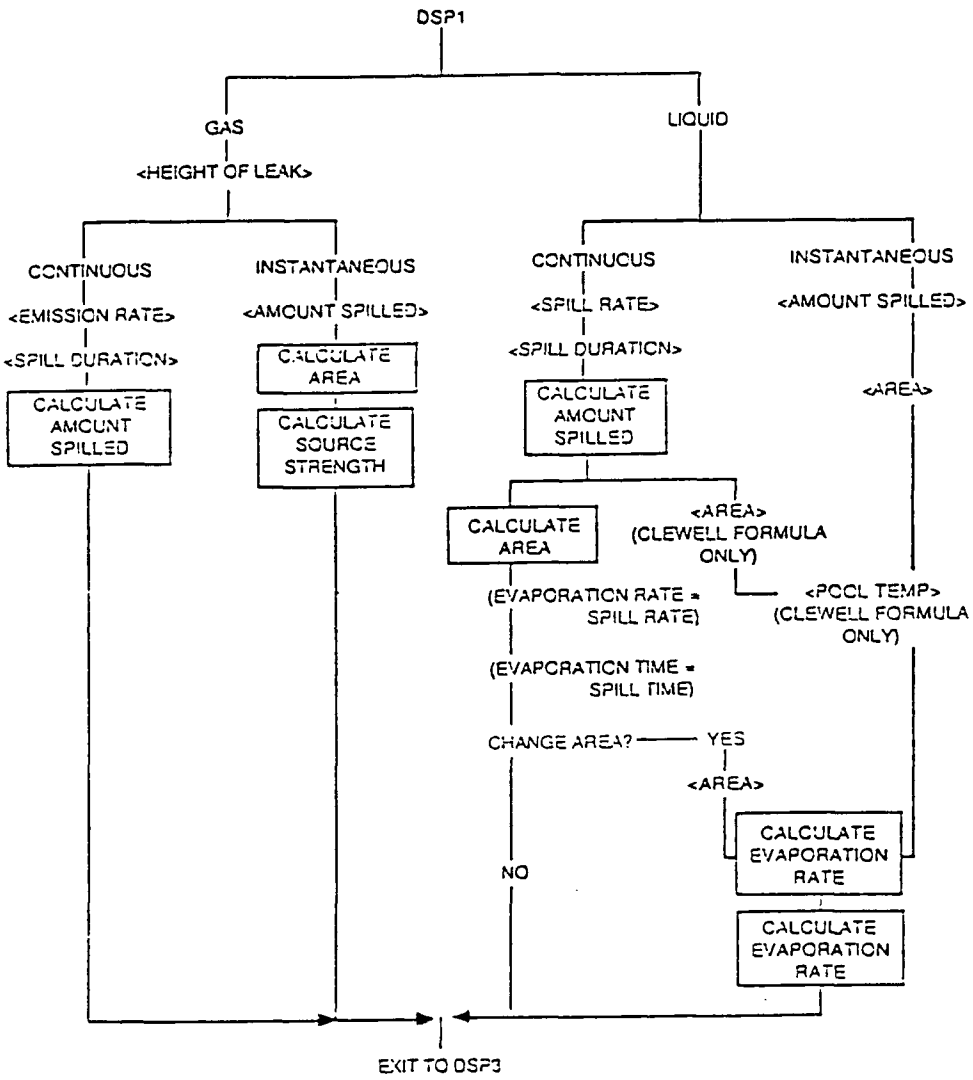
APPENDIX A

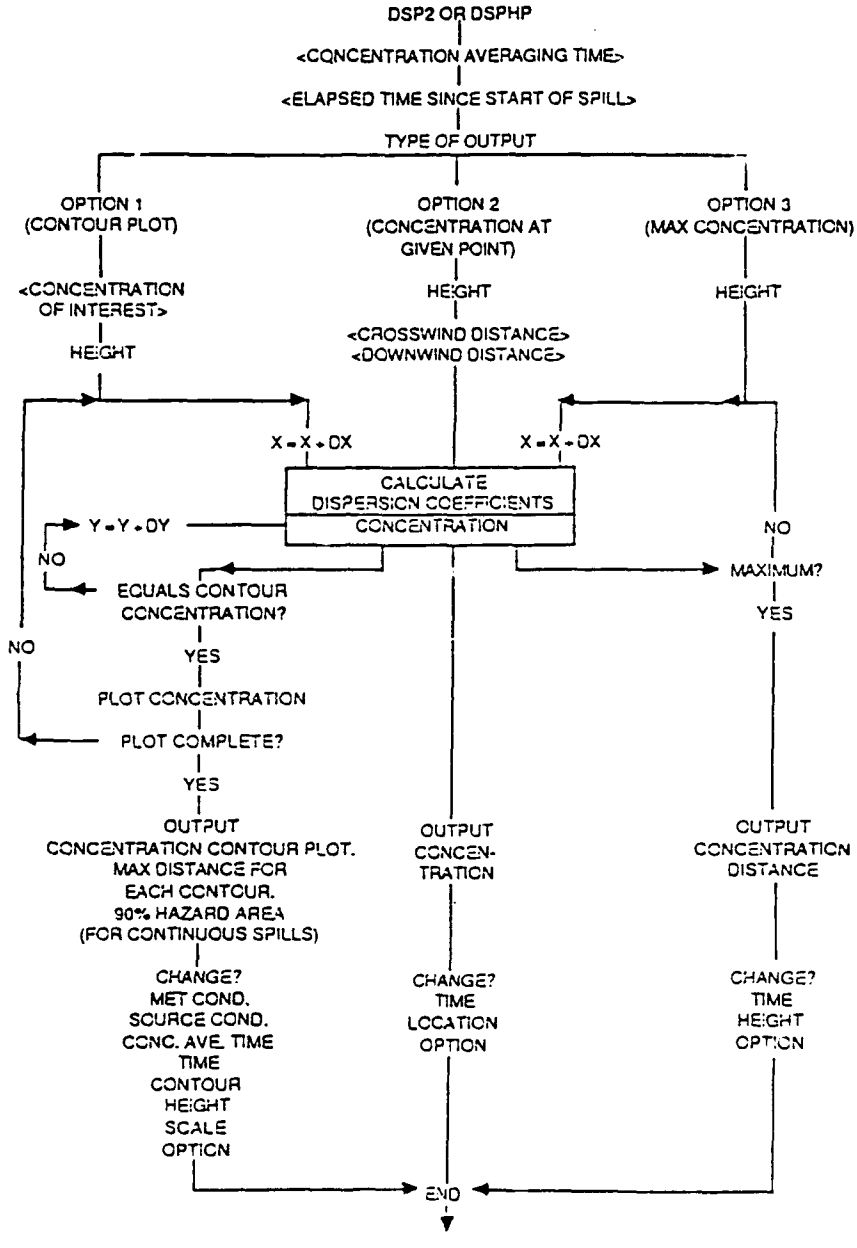
AFTOX Flow Charts



DSP1 Flow Diagram



DSP2 Flow Diagram



DSP3 Flow Diagram

APPENDIX B

Partial Derivatives

The following is a list of the needed partial derivatives taken from AFTOX's Gaussian puff equation. For ease in derivation, the following shorthand notation is used:

$$M = Q(t')/(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z$$

$$N = \exp\{-(x-u(t-t'))^2/2\sigma_x^2\}$$

$$O = \exp\{-y^2/2\sigma_y^2\}$$

$$P = \exp\{-(z-h)^2/2\sigma_z^2\}+\exp\{-(z+h)^2/2\sigma_z^2\}$$

$$A = \exp\{-(z-h)^2/2\sigma_z^2\}$$

$$B = \exp\{-(z+h)^2/2\sigma_z^2\}$$

where the concentration $G(x,y,z,t-t') = MNOP$.

The following simplifications are also used:

$$CZ = A\cdot(z-h)^2/\sigma_z^3 + B\cdot(z+h)^2/\sigma_z^3$$

$$CZ1 = A\cdot(z-h)/\sigma_z^2 - B\cdot(z+h)/\sigma_z^2$$

$$CT = x-u(t-t')$$

$$CT2 = (x-u(t-t'))(t-t')/\sigma_x^2$$

$$CT3 = (x-u(t-t'))^2/\sigma_x^3$$

$$YT1 = y^2/\sigma_y^2$$

First order partial derivatives:

$$\delta G/\delta Q = G/Q \qquad \delta G/\delta u = G \cdot CT2$$

$$\delta G/\delta \sigma_x = -G/\sigma_x + G \cdot CT3 \qquad \delta G/\delta \sigma_y = -G/\sigma_y + G \cdot YT1/\sigma_y$$

$$\delta G/\delta \sigma_z = -G/\sigma_z + MNO \cdot CZ \qquad \delta G/\delta h = MNO \cdot CZ1$$

Cross-partial derivatives:

$$\delta^2 G/\delta Q \delta u = (\delta G/\delta Q) \cdot CT2$$

$$\delta^2 G/\delta Q \delta \sigma_x = \{(\delta G/\delta Q) \cdot CT3\} - \{(\delta G/\delta Q)/\sigma_x\}$$

$$\delta^2 G/\delta Q \delta \sigma_y = \{(\delta G/\delta Q) \cdot YT1\} - \{(\delta G/\delta Q)/\sigma_y\}$$

$$\delta^2 G/\delta Q \delta \sigma_z = \{(MNO/Q) \cdot CZ\} - \{(\delta G/\delta Q)/\sigma_z\}$$

$$\delta^2 G/\delta Q \delta h = (MNO/Q) \cdot CZ1$$

$$\delta^2 G/\delta u \delta \sigma_x = (-G/\sigma_x) \cdot CT2 + G \cdot \{CT3 \cdot (t-t') - 2 \cdot CT \cdot (t-t')/\sigma_x^3\}$$

$$\delta^2 G/\delta u \delta \sigma_y = (\delta G/\delta \sigma_y) \cdot CT2$$

$$\delta^2 G/\delta u \delta \sigma_z = (\delta G/\delta \sigma_z) \cdot CT2$$

$$\delta^2 G/\delta u \delta h = (\delta G/\delta h) \cdot CT2$$

$$\delta^2 G/\delta \sigma_x \delta \sigma_y = (-G/\sigma_x) \cdot YT1 + G/\sigma_x \sigma_y - (G/\sigma_y) \cdot CT3 + G \cdot CT3 \cdot YT1$$

$$\delta^2 G/\delta \sigma_x \delta \sigma_z = (-G/\sigma_z) \cdot CT3 + G/\sigma_x \sigma_z - (MNO/\sigma_x) \cdot CZ + MNO \cdot CT3 \cdot CZ$$

$$\delta^2 G/\delta \sigma_x \delta h = (-MNO/\sigma_x) \cdot CZ1 + MNO \cdot CT3 \cdot CZ1$$

$$\delta^2 G/\delta \sigma_y \delta \sigma_z = (-G/\sigma_z) \cdot YT1 + G/\sigma_y \sigma_z - (MNO/\sigma_y) \cdot CZ + MNO \cdot YT1 \cdot CZ$$

$$\delta^2 G/\delta \sigma_y \delta h = (-MNO/\sigma_y) \cdot CZ1 + MNO \cdot YT1 \cdot CZ1$$

$$\delta^2 G/\delta\sigma_z\delta h = MNO\cdot\{A\cdot(z-h)^3/\sigma_z^5 - 2A\cdot(z-h)/\sigma_z^3 - B\cdot(z+h)^3/\sigma_z^5 + 2B\cdot(z+h)/\sigma_z^3\} - \{(MNO/\sigma_z)\cdot CZ1\}$$

Second-order partial derivatives:

$$\delta^2 G/\delta Q^2 = 0$$

$$\delta^2 G/\delta u^2 = G\cdot\{CT2^2 - (t-t')^2/\sigma_x^2\}$$

$$\delta^2 G/\delta\sigma_x^2 = G\cdot\{2/\sigma_x^2 - 2\cdot CT3/\sigma_x + CT3^2 - 3\cdot CT3/\sigma_x\}$$

$$\delta^2 G/\delta\sigma_y^2 = G\cdot\{2/\sigma_y^2 - 2\cdot YT1/\sigma_y + YT1^2 - 3\cdot YT1/\sigma_y\}$$

$$\delta^2 G/\delta\sigma_z^2 = 2G/\sigma_z^2 - 2MNO\cdot CZ/_z + MNO\cdot\{A\cdot[(z-h)^4/\sigma_z^6 - 3(z-h)^2/\sigma_z^4] + B\cdot[(z+h)^4/\sigma_z^6 - 3(z+h)^2/\sigma_z^4]\}$$

$$\delta^2 G/\delta h^2 = MNO\cdot\{A\cdot[(z-h)^2/\sigma_z^4 - 1/\sigma_z^2] + B\cdot[(z+h)^2/\sigma_z^4 - 1/\sigma_z^2]\}$$